Influence of Constitution and Charge on Radical Pairing Interactions in Trisradical Tricationic Complexes

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SUPPORTING INFORMATION

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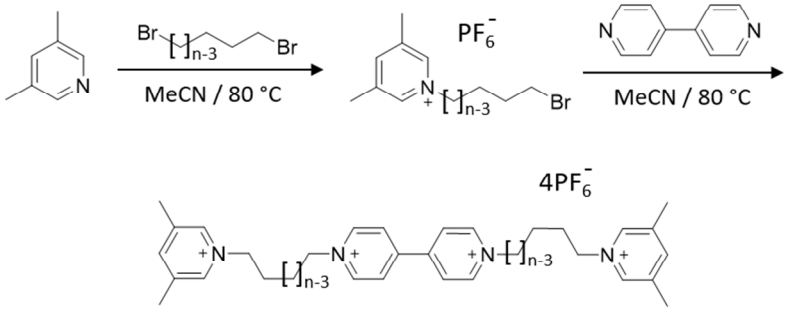
1. General Methods

All reagents were purchased from commercial suppliers (Sigma-Aldrich or Fisher) and employed without further purification. Cyclobis(paraquat-*p*-phenylene) tetrakis(hexafluorophosphate)[1] (CBPQT•4PF_6), DB1•2PF_6[2], DB7•2PF_6[3], S1•2PF_6[4], S2•PF_6[4], S3•PF_6[3], S4[5] S6•2PF_6[6] were prepared according to literature procedures. Thin layer chromatography (TLC) was performed on silica gel 60 F254 (E. Merck). Column chromatography was carried out on silica gel 60F (Merck 9385, 0.040–0.063 mm). Solvents used in experiments involving radicals were degassed using the freeze-pump-thaw method. UV-Vis-NIR Spectra were recorded on a Varian 100-Bio UV-Vis spectrophotometer in MeCN at room temperature. Nuclear magnetic resonance (NMR) spectra were recorded on Bruker Avance 600 or Varian P-Inova 500 spectrometers, with working frequencies of 600 and 500 MHz for ^{1}H, and 150 and 125 MHz for ^{13}C nuclei, respectively. Chemical shifts are reported in ppm relative to the signals corresponding to the residual non-deuterated solvents ($CHCl_3$: δ = 7.26 ppm, CD_2HCN: δ =1.94 ppm). High resolution mass spectra were measured on a Finnigan LCQ iontrap mass spectrometer (HR-ESI). Cyclic voltammetry (CV) experiments were carried out at room temperature in argon-purged MeCN solutions with a Gamry Multipurpose instrument (Reference 600) interfaced to a PC. CV Experiments were performed using a glassy carbon working electrode (0.071 cm^2). The electrode surface was polished routinely with 0.05 μm alumina-water slurry on a felt surface immediately before use. The counter electrode was a Pt coil and the reference electrode was Ag/AgCl electrode. The concentration of supporting electrolyte (tetrabutylammonium hexafluorophosphate) was 0.1 M.

2. Synthetic Procedures



	n
DB2•4PF_6	11
DB3•4PF_6	8
DB4•4PF_6	6
DB5•4PF_6	5
DB6•4PF_6	4

Scheme S1. General Synthesis of **DB2-6**•4PF_6

General Procedure for DB2-6•4PF_6: A mixture of 3,5-lutidine (10 mmol) and the appropriate α,ω-dibromoalkane (100 mmol) was dissolved in MeCN (50 mL) and stirred at 80 °C overnight. After cooling to room temperature, the reaction mixture was poured into Et_2O (200 mL). The resulting suspension was extracted with H_2O (3 × 100 mL) and then NH_4PF_6 (3 g) was added to the combined aqueous phase. The precipitate was filtered and washed with H_2O (3 x 10 mL) to afford the appropriate precursors. A mixture of 4,4′-bipyridine (2 mmol) and the appropriate precursors (5 mmol) was stirred in MeCN (10 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB2-6•4PF_6 as white solid.

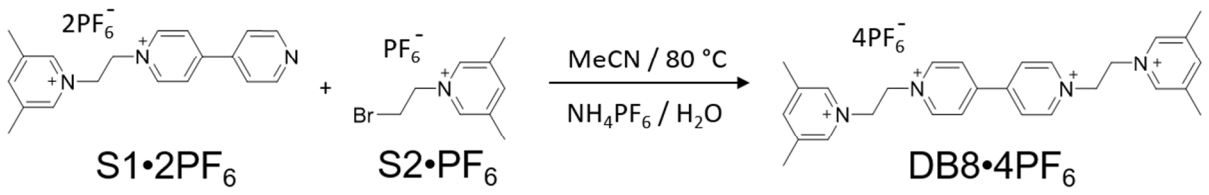
DB2•4PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.90 (d, *J* = 7.0 Hz, 4H), 8.38 (d, *J* = 6.8 Hz, 4H), 8.34 (s, 4H), 8.12 (s, 2H), 4.60 (t, *J* = 7.5 Hz, 4H), 4.37 (t, *J* = 7.5 Hz, 4H), 2.46 (s, 12H), 2.05 – 1.95 (m, 4H), 1.93 – 1.89 (m, 4H), 1.43 – 1.23 (m, 28H). ^{13}C NMR (126 MHz, CD_3CN) δ 149.5, 146.2, 145.2, 140.8, 138.6, 126.8, 61.7, 61.1, 30.7, 30.4, 28.8, 28.8, 28.7, 28.4, 28.3, 25.3, 25.3, 17.0. ESI-HRMS calcd for *m/z* = 1113.4520 $[M - PF_6]^+$, found *m/z* = 1113.4532.

DB3•4PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.89 (d, *J* = 7.0 Hz, 4H), 8.37 (d, *J* = 6.3 Hz, 4H), 8.33 (s, 4H), 8.13 (s, 2H), 4.59 (t, *J* = 7.4 Hz, 4H), 4.38 (t, *J* = 7.6 Hz, 4H), 2.46 (s, 12H), 2.04 – 1.97 (m, 4H), 1.93 – 1.89 (m, 4H), 1.41 – 1.31 (m, 16H).^{13}C NMR (126 MHz, CD_3CN) δ 149.5, 146.2, 145.2, 140.8, 138.6, 126.8, 61.7, 61.1, 30.6, 30.3, 28.0, 28.0, 25.2(2C), 17.0. ESI-HRMS calcd for *m/z* = 1029.3581 $[M - PF_6]^+$, found *m/z* = 1029.3607.

DB4•4PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.89 (d, *J* = 6.9 Hz, 4H), 8.38 (d, *J* = 6.4 Hz, 4H), 8.34 (s, 4H), 8.14 (s, 2H), 4.60 (t, *J* = 7.5 Hz, 4H), 4.39 (t, *J* = 7.6 Hz, 4H), 2.04 – 1.98 (m, 4H), 1.98 – 1.92 (m, 4H), 1.47 – 1.36 (m, 8H). ^{13}C NMR (126 MHz, CD_3CN) δ 149.6, 146.2, 145.2, 140.9, 138.7, 126.8, 61.5, 60.9, 30.2, 30.0, 24.6, 24.6, 17.0. ESI-HRMS calcd for *m/z* = 973.2955 $[M - PF_6]^+$, found *m/z* = 973.2975.

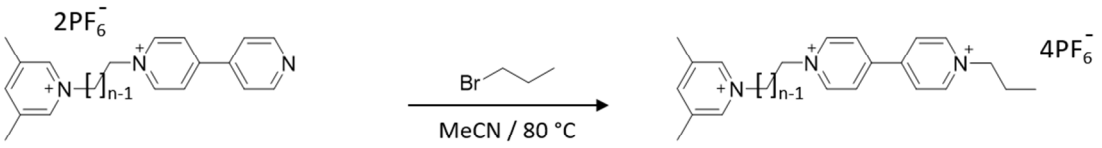
DB5•4PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.90 (d, *J* = 6.9 Hz, 4H), 8.40 (d, *J* = 6.3 Hz, 4H), 8.35 (s, 4H), 8.15 (s, 2H), 4.61 (t, *J* = 7.6 Hz, 4H), 4.40 (t, *J* = 7.5 Hz, 4H), 2.48 (s, 12H), 2.10 – 1.97 (m, 8H), 1.49 – 1.40 (m, 4H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.6, 147.3, 146.2, 141.8, 139.7, 127.8, 62.2, 61.5, 30.7, 30.5, 22.7, 17.9. ESI-HRMS calcd for *m/z* = 945.2642 $[M - PF_6]^+$, found *m/z* = 945.2668.

DB6•4PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.90 (d, *J* = 6.9 Hz, 4H), 8.42 (d, *J* = 6.6 Hz, 4H), 8.36 (s, 4H), 8.19 (s, 2H), 4.66 (t, *J* = 7.5 Hz, 4H), 4.48 (t, *J* = 7.5 Hz, 4H), 2.50 (s, 12H), 2.08 – 2.05 (m, 8H). ^{13}C NMR (126 MHz, CD_3CN) δ 149.7, 146.5, 145.3, 140.9, 138.8, 126.9, 60.7, 60.1, 27.0, 26.7, 17.0. ESI-HRMS calcd for *m/z* = 917.2329 $[M - PF_6]^+$, found *m/z* = 917.2344.



Scheme S2. Synthesis of DB8•4PF_6

DB8•4PF_6: A mixture of S1•2PF_6 (100 mg, 0.17 mmol) and S2•PF_6 (100 mg, 0.26 mmol) was stirred in MeCN (1 mL) at 80 °C for 7 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB8•4PF_6 (45 mg, 25%) as a white solid. ^{1}H NMR (500 MHz, CD_3CN) δ 8.86 (d, *J* = 6.9 Hz, 4H), 8.45 (d, *J* = 6.9 Hz, 4H), 8.37 (s, 4H), 8.27 (s, 2H), 5.17 (t, *J* = 6.6 Hz, 4H), 5.01 (t, *J* = 6.6 Hz, 4H), 2.49 (s, 12H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.6, 148.1, 145.9, 141.4, 139.6, 127.7, 59.6, 59.0, 17.1. ESI-HRMS calcd for *m/z* = 861.1703 $[M - PF_6]^+$, found *m/z* = 861.1712.



	n
S1•2PF_6	2
S3•2PF_6	3

	n
DB9•4PF_6	2
DB10•4PF_6	3

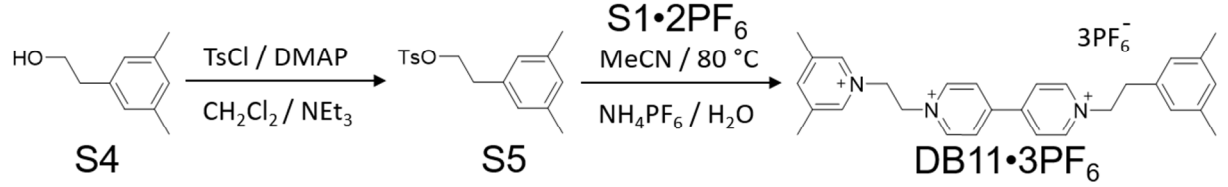
Scheme S3. General Synthesis of DB9•4PF_6 and DB10•4PF_6

General Procedure for DB9•3PF_6 and DB10•3PF_6: A mixture of S1•2PF_6 or S3•2PF_6 (0.17 mmol) and 1-bromopropane (1 mmol) was stirred in MeCN (1 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting reaction mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ =

7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB9•3PF_6 or DB10•3PF_6 as a white solid.

DB9•3PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.94 (d, *J* = 6.4 Hz, 2H), 8.82 (d, *J* = 7.0 Hz, 2H), 8.45 (d, *J* = 6.9 Hz, 2H), 8.41 (d, *J* = 6.2 Hz, 2H), 8.36 (s, 2H), 8.30 (s, 1H), 5.17 (t, *J* = 6.5 Hz, 2H), 5.02 (t, *J* = 6.6 Hz, 2H), 4.64 (t, *J* = 7.4 Hz, 2H), 2.51 (s, 6H), 2.13 – 2.04 (m, 2H), 1.04 (t, *J* = 7.3 Hz, 2H). ^{13}C NMR (126 MHz, CD_3CN) δ 152.0, 150.1, 149.0, 146.7, 146.2, 142.3, 140.6, 128.5, 127.9, 64.1, 60.5, 59.9, 25.0, 18.0, 10.1. ESI-HRMS calcd for *m/z* = 624.1566 $[M - PF_6]^+$, found *m/z* = 624.1572.

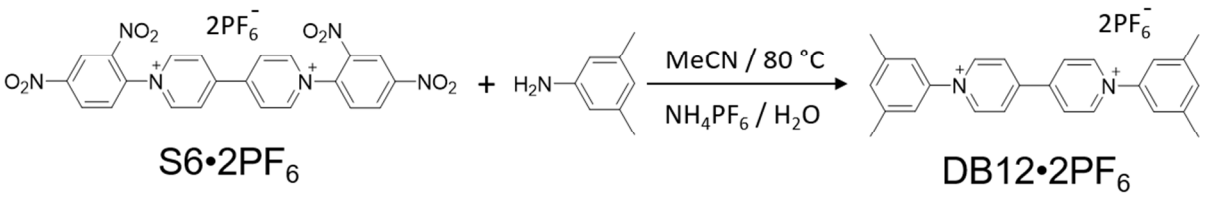
DB10•3PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.95 – 8.89 (m, 4H), 8.45 (d, *J* = 6.6 Hz, 2H), 8.42 – 8.39 (m, 4H), 8.24 (s, 1H), 4.72 (t, *J* = 7.8 Hz, 2H), 4.63 (t, *J* = 7.4 Hz, 2H), 4.58 (t, *J* = 7.5 Hz, 2H), 2.73 – 2.63 (m, 2H), 2.53 (s, 6H), 2.13 – 2.04 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (126 MHz, CD_3CN) δ 151.2, 150.4, 147.8, 146.3, 146.2, 142.0, 140.1, 128.1, 127.8, 64.0, 58.9, 58.2, 32.2, 25.0, 18.0, 10.1. ESI-HRMS calcd for *m/z* = 638.1718 $[M - PF_6]^+$, found *m/z* = 638.1726.



Scheme S4. Synthesis of DB11•3PF_6

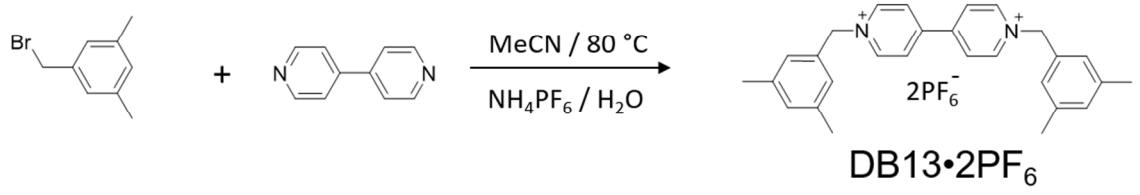
DB11•3PF_6: A mixture of **S4** (1.0 g, 6.7 mmol), TsCl (1.5 g, 7.9 mmol) and DMAP (50 mg) was stirred in CH_2Cl_2 (40 mL) and NEt_3 (10 mL) for 3 h. The reaction was quenched by adding H_2O (50 mL), followed by extraction with CH_2Cl_2 (3×40 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$), concentrated under vacuum and then purified column chromatography (SiO_2 : Hexanes / EtOAc = 10:1) to afford **S5** (1.52 g, 76%) as a colorless oil. ^{1}H NMR (500 MHz, CD_3CN) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 6.84 (s, 1H), 6.70 (s, 2H), 4.18 (t, *J* = 7.2 Hz, 2H), 2.87 (t, *J* = 7.2 Hz, 2H), 2.43 (s, 3H), 2.24 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.6, 138.1, 136.0, 133.0, 129.7, 128.5, 127.9, 126.7, 70.8, 35.2, 21.7, 21.2. A mixture of **S5** (100 mg, 0.33 mmol) and S1•2PF_6 (100 mg, 0.17 mmol) was stirred in MeCN (1 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 :

MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB11•3PF_6 (110 mg, 74%) as a white solid. ^{1}H NMR (500 MHz, CD_3CN) δ 8.85 – 8.80 (m, 2H), 8.76 (d, *J* = 6.9 Hz, 2H), 8.43 (d, *J* = 7.0 Hz, 2H), 8.37 (s, 2H), 8.33 (d, *J* = 6.3 Hz, 2H), 8.30 (s, 1H), 6.98 (s, 1H), 6.81 (s, 2H), 5.17 (t, *J* = 6.5 Hz, 2H), 5.02 (t, *J* = 6.5 Hz, 2H), 4.88 (t, *J* = 7.1 Hz, 2H), 3.28 (t, *J* = 7.1 Hz, 2H), 2.51 (s, 6H), 2.27 (s, 6H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.9, 149.2, 148.1, 145.8, 145.3, 141.4, 139.7, 138.4, 134.8, 128.6, 127.6, 126.6, 126.2, 62.7, 59.6, 59.0, 36.3, 19.9, 17.1. ESI-HRMS calcd for *m/z* = 714.2031 $[M - PF_6]^+$, found *m/z* = 714.2040.



Scheme S5. Synthesis of DB12•2PF_6

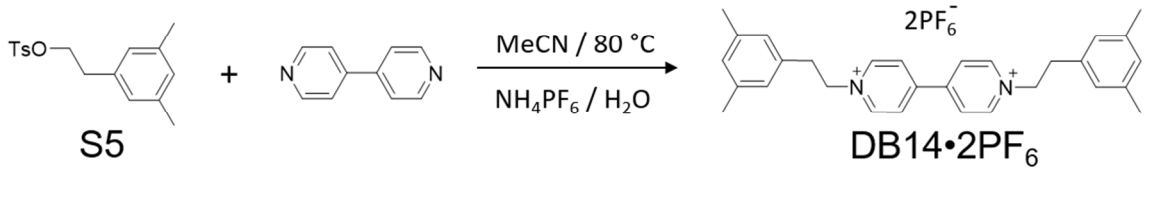
DB12•2PF_6: A mixture of S6•2PF_6 (1.0 g, 1.3 mmol) and 3,5-dimethylaniline (0.5 g, 4.1 mmol) was stirred in MeCN (10 mL) at 80 °C overnight. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB12•2PF_6 (600 mg, 70%) as a red solid. ^{1}H NMR (500 MHz, CD_3CN) δ 9.16 (d, *J* = 7.1 Hz, 4H), 8.62 (d, *J* = 6.9 Hz, 4H), 7.46 (s, 2H), 7.42 (s, 4H), 2.49 (s, 12H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.7, 146.0, 142.9, 141.8, 134.0, 127.8, 122.5, 20.8. ESI-HRMS calcd for *m/z* = 511.1732 $[M - PF_6]^+$, found *m/z* = 511.1735.



Scheme S6. Synthesis of DB13•2PF_6

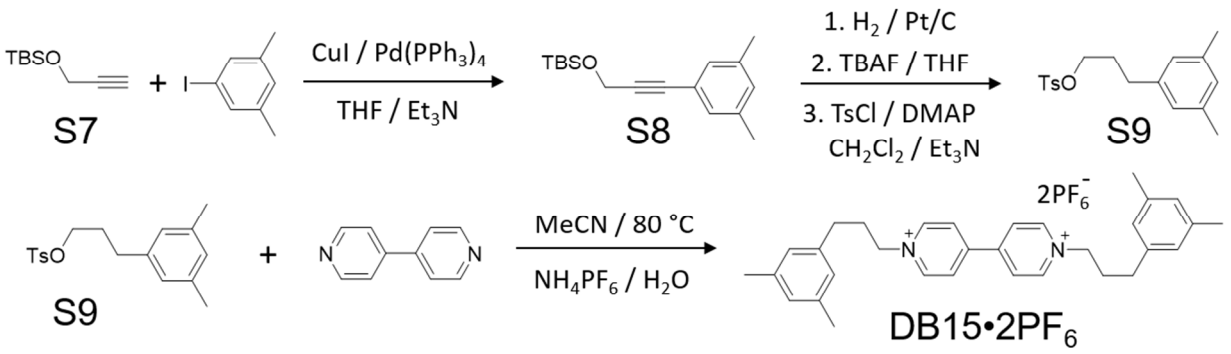
DB13•2PF_6: A mixture of 3,5-dimethylbenzylbromide (1.5 g, 7.5 mmol) and 4,4′-bipyridine (500 mg, 3.3 mmol) was stirred in MeCN (10 mL) at 80 °C for 2 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by

column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB13•2PF_6 (2.07 mg, 92%) as a white solid. ^{1}H NMR (500 MHz, CD_3CN) δ 8.94 (d, J = 6.9 Hz, 4H), 8.34 (d, J = 6.6 Hz, 4H), 7.14 (s, 2H), 7.11 (s, 4H), 5.72 (s, 4H), 2.32 (s, 12H). ^{13}C NMR (126 MHz, CD_3CN) δ 147.4, 146.1, 140.1, 133.0, 132.0, 128.0, 127.5, 65.4, 20.8. ESI-HRMS calcd for m/z = 539.2045 [M – PF_6]$^+$, found m/z = 539.2043.



Scheme S7. Synthesis of DB14•2PF_6

DB14•2PF_6: A mixture of S5 (300 mg, 1.0 mmol) and 4,4′-bipyridine (50 mg, 0.33 mmol) was stirred in MeCN (1 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB14•2PF_6 (176 mg, 76%) as a white solid. ^{1}H NMR (500 MHz, CD_3CN) δ 8.72 (d, J = 6.9 Hz, 2H), 8.30 (d, J = 6.3 Hz, 2H), 6.97 (s, 1H), 6.79 (s, 2H), 4.85 (t, J = 7.1 Hz, 2H), 3.26 (t, J = 7.1 Hz, 2H), 2.26 (s, 6H). ^{13}C NMR (126 MHz, CD_3CN) δ 149.5, 145.1, 138.4, 134.8, 128.6, 126.5, 126.2, 62.7, 36.3, 19.9. ESI-HRMS calcd for m/z = 567.2358 [M – PF_6]$^+$, found m/z = 567.2360.

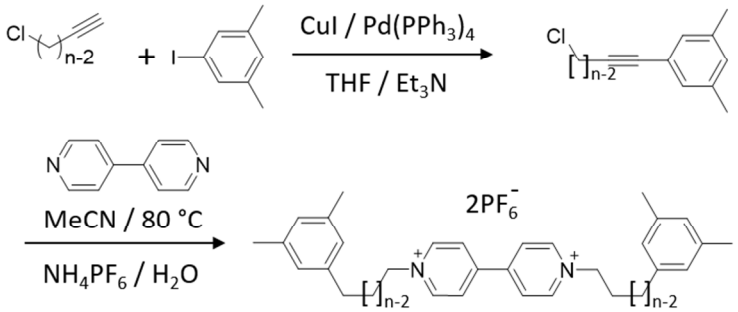


Scheme S8. Synthesis of DB15•2PF_6

DB15•2PF_6: A mixture of 1-iodo-3,5-dimethylbenzene (1.0 g, 4.3 mmol), S7 (0.88g, 5.2 mmol), copper(I) iodide (40 mg, 0.21 mmol) and tetrakis(triphenylphosphine)palladium(0) (80 mg, 0.07

mmol) was stirred in THF (10 mL) and Et_3N (5 mL) under N_2 at room temperature overnight. The reaction was quenched by adding H_2O (50 mL), followed by extraction with CH_2Cl_2 (3×40 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$), concentrated under vacuum and then purified column chromatography (SiO_2 : Hexanes / CH_2Cl_2 = 10:1) to afford **S8** (0.98 g, 83%) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.05 (d, *J* = 1.6 Hz, 2H), 6.94 (s, 1H), 4.53 (s, 2H), 2.28 (s, 6H), 0.94 (s, 9H), 0.17 (s, 6H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.8, 130.2, 129.3, 122.6, 87.1, 85.1, 52.3, 25.9, 21.1, 18.4 , -5.0. The alkyne (0.98 g, 3.6 mmol) was stirred under H_2 in THF (50 mL) with platinum on activated carbon (100 mg) overnight. TBAF (3.6 mL, 1M in THF) was added to the solution after filtration. The mixture was stirred for another 1 h at room temperature. The reaction was quenched by adding H_2O (50 mL), followed by extraction with CH_2Cl_2 (3×40 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$), concentrated under vacuum and then purified column chromatography (SiO_2 : Hexanes / EtOAc = 4:1) to afford a colorless oil. The oil was dissolved in CH_2Cl_2 (10 mL) and Et_3N (1 mL) and stirred with DMAP (50 mg) and TsCl (700 mg, 3.7 mmol) at room temperature for 3 h. The reaction was quenched by adding H_2O (50 mL), followed by extraction with CH_2Cl_2 (3×40 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$), concentrated under vacuum and then purified column chromatography (SiO_2 : Hexanes / EtOAc = 10:1) to afford **S9** (740 mg, 65% for 3 steps) as a colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 6.82 (s, 1H), 6.69 (d, *J* = 1.5 Hz, 2H), 4.04 (t, *J* = 6.2 Hz, 2H), 2.61 – 2.51 (m, 2H), 2.45 (s, 3H), 2.25 (s, 6H), 2.01 – 1.84 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.7, 140.3, 138.0, 133.2, 129.8, 127.9, 127.8, 126.3, 69.8, 31.3, 30.5, 21.7, 21.2. A mixture of **S9** (500 mg, 1.6 mmol) and 4,4′-bipyridine (100 mg, 0.67 mmol) was stirred in MeCN (1 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB15•2PF_6 (416 mg, 83%) as a white solid. ^{1}H NMR (500 MHz, CD_3CN) δ 8.84 (d, *J* = 6.3 Hz, 4H), 8.27 (d, *J* = 6.3 Hz, 4H), 6.84 (s, 2H), 6.81 (s, 4H), 4.65 (t, *J* = 7.3 Hz, 4H), 2.69 (t, *J* = 7.6 Hz, 4H), 2.35 (t, *J* = 7.4 Hz, 4H), 2.23 (s, 12H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.3, 146.2, 140.5, 138.8, 128.3, 127.4, 126.6, 62.5, 32.4, 32.2, 20.9. ESI-HRMS calcd for *m/z* = 595.2671 $[M - PF_6]^+$, found *m/z* = 595.2668.

General Procedure for DB16-18•2PF$_6$: A mixture of 1-iodo-3,5-dimethylbenzene (1.0 g, 4.3 mmol), the appropriate terminal alkyne chloride (5.0 mmol), copper(I) iodide (40 mg, 0.21 mmol) and tetrakis(triphenylphosphine)palladium(0) (80 mg, 0.07 mmol) was stirred in THF (10 mL) and Et_3N (5 mL) under N_2 at room temperature overnight. The reaction was quenched by adding H_2O (50 mL), followed by extraction with CH_2Cl_2 (3×40 mL). The combined organic phase was washed with brine (50 mL), dried ($MgSO_4$), concentrated under vacuum and then purified column chromatography (SiO_2 : Hexanes / CH_2Cl_2 = 10:1) to afford corresponding alkyne. The alkynes are dissolved in THF (50 mL) with platinum on activated carbon (100 mg) and stirred overnight under H_2. The appropriate chloride was afforded after removal of the solvent under vacuum. A mixture of 4,4′-bipyridine (100 mg, 0.67 mmol) and the appropriate chloride (1.5 mmol) was stirred in MeCN (1 mL) at 80 °C for 3 days. After cooling to room temperature, the solvent was removed in vacuum, and the resulting mixture was purified by column chromatography (SiO_2 : MeOH / NH_4Cl (aq, 2M) / $MeNO_2$ = 7:2:1), followed by counterion exchange (NH_4PF_6 / H_2O) to afford DB16-18•2PF$_6$.



	n
DB16•2PF$_6$	4
DB17•2PF$_6$	5
DB18•2PF$_6$	6

Scheme S9. General Synthesis of DB16-18•4PF$_6$

DB16•2PF$_6$: ^{1}H NMR (500 MHz, CD_3CN) δ 8.86 (d, *J* = 6.7 Hz, 4H), 8.35 (d, *J* = 6.2 Hz, 4H), 6.85 (s, 2H), 6.81 (s, 4H), 4.62 (t, *J* = 7.4 Hz, 4H), 2.60 (t, *J* = 7.6 Hz, 4H), 2.25 (s, 12H), 2.06 – 1.98 (m, 4H), 1.73 – 1.57 (m, 4H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.5, 146.1, 142.1, 138.5, 128.0, 127.8, 126.7, 62.6, 35.1, 31.2, 28.0, 20.9. ESI-HRMS calcd for *m/z* = 623.2984 [*M* – PF_6]$^+$, found *m/z* = 623.2983.

DB17•2PF$_6$: ^{1}H NMR (500 MHz, CD_3CN) δ 8.91 (d, *J* = 6.8 Hz, 4H), 8.39 (d, *J* = 6.3 Hz, 4H), 6.92 – 6.79 (m, 6H), 4.64 (t, *J* = 7.6 Hz, 4H), 2.58 (t, *J* = 7.7 Hz, 4H), 2.28 (s, 12H), 2.11 – 2.03 (m, 4H), 1.75 – 1.60 (m, 4H), 1.56 – 1.38 (m, 4H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.4, 146.1, 142.8, 138.3, 127.8, 127.7, 126.7, 62.5, 35.5, 31.3, 31.0, 25.7, 20.9. ESI-HRMS calcd for *m/z* =

651.3297 $[M - PF_6]^+$, found *m/z* = 651.3293.

DB18•2PF_6: ^{1}H NMR (500 MHz, CD_3CN) δ 8.91 (d, *J* = 6.9 Hz, 4H), 8.39 (d, *J* = 6.2 Hz, 6H), 6.96 – 6.74 (m, 7H), 4.63 (t, *J* = 7.6 Hz, 5H), 2.56 (t, *J* = 7.7 Hz, 5H), 2.28 (s, 13H), 2.09 – 2.01 (m, 5H), 1.67 – 1.58 (m, 5H), 1.47 – 1.39 (m, 10H). ^{13}C NMR (126 MHz, CD_3CN) δ 150.4, 146.1, 143.1, 138.3, 127.7, 127.7, 126.7, 62.7, 35.7, 31.6, 31.4, 28.8, 26.0, 20.9. ESI-HRMS calcd for *m/z* = 679.3610 $[M - PF_6]^+$, found *m/z* = 679.3609.

3. Binding Constant Measurements

General Experiment Method: A MeCN solution of CBPQT•4PF_6 (~2 mL, 5.0 × 10^{-4} M unless stated otherwise) was added to an excess of activated Zn dust and the reaction mixture was stirred in glovebox for 5 min. An MeCN solution of DB1•2PF_6, DB2–7•4PF_6, DB8–10•3PF_6, or DB11–18•2PF_6 (∼3.0 × 10^{-2} M unless stated otherwise) was titrated into $CBPQT^{2(\bullet+)}$ solution. After each titration, the mixture was stirred for 1 min, after which a 0.35 mL aliquot of the reaction mixture was filtered and sealed in a 1 mm UV cuvette. Vis/NIR spectra were recorded from 1500 to 450 nm and the cuvette was returned into glovebox. The combined reaction mixture was titrated again until the trisradical band (~1080 nm) reached saturation (4~8 equiv of the dumbbells).

General Data Analysis Method:

$$V^{\bullet+} + CBPQT^{2(\bullet+)} \rightleftharpoons V^{\bullet+}\subset CBPQT^{2(\bullet+)}$$

	$V^{\bullet+}$	$CBPQT^{2(\bullet+)}$	$V^{\bullet+}\subset CBPQT^{2(\bullet+)}$
Initial Concentration	c_V	c_{CBPQT}	0
Equilibrium Concentration	$[c_V]$	$[c_{CBPQT}]$	$[c]$

The binding constant *K* can be expresed as follows –

$$K = \frac{[c]}{[c_V][c_{CBPQT}]} \quad (1)$$

According to the stoichiometry governing the chemical equilibrium and ignoring the volume change during the titrations, we have –

$$[c] = c_{CBPQT} - [c_{CBPQT}] \quad (2)$$

$$[c] = c_V - [c_V] \quad (3)$$

Let –

$$x = c_V / c_{CBPQT} \quad (4)$$

Substituting Equations (2), (3) and (4) into Equation (1) and rearranging gives –

$$[c] = \frac{1}{2K} + \frac{c_{\mathrm{CBPQT}}}{2}(x+1) - \frac{1}{2}\sqrt{(c_{\mathrm{CBPQT}}x)^2 + \left(\frac{2c_{\mathrm{CBPQT}}}{K} - 2c_{\mathrm{CBPQT}}^2\right)x + (c_{\mathrm{CBPQT}} + \frac{1}{K})^2} \quad (5)$$

The trisradical band of $V^{\bullet+}\subset CBPQT^{2(\bullet+)}$ observed around 1080 nm has no overlap with other peaks and so we can apply the Beer–Lambert law, where ε is molar attenuation coefficient and l is light path length –

$$A = \varepsilon\, l\, [c] \quad (6)$$

When the dumbbell / $CBPQT^{2(\bullet+)}$ ratio x approaches infinity –

$$\lim_{x\to\infty}[c] = c_{\mathrm{CBPQT}} \quad (7)$$

Substituting Equation (7) into Equation (6) gives –

$$A_{\mathrm{sat}} = \varepsilon\, l\, c_{\mathrm{CBPQT}} \quad (8)$$

Substituting Equation (8) back to equation (6) eliminates ε and l affording –

$$A = A_{sat}[c]/c_{\mathrm{CBPQT}} \quad (9)$$

Combining Equation (5) and (9), where c_{CBPQT} is the known initial CBPQT•$4PF_6$ concentration, x is the known titrated dumbbell equiv, and A is the experimentally measured absorption of trisradial band, we can fit the experiment data to solve the unknown constants K and A_{sat} by varying x and the dependent variable A. The original titration UV/Vis/NIR spectra and titration curves are presented in **Figure S1**–**S20**. The results are summarized in **Table S1**.

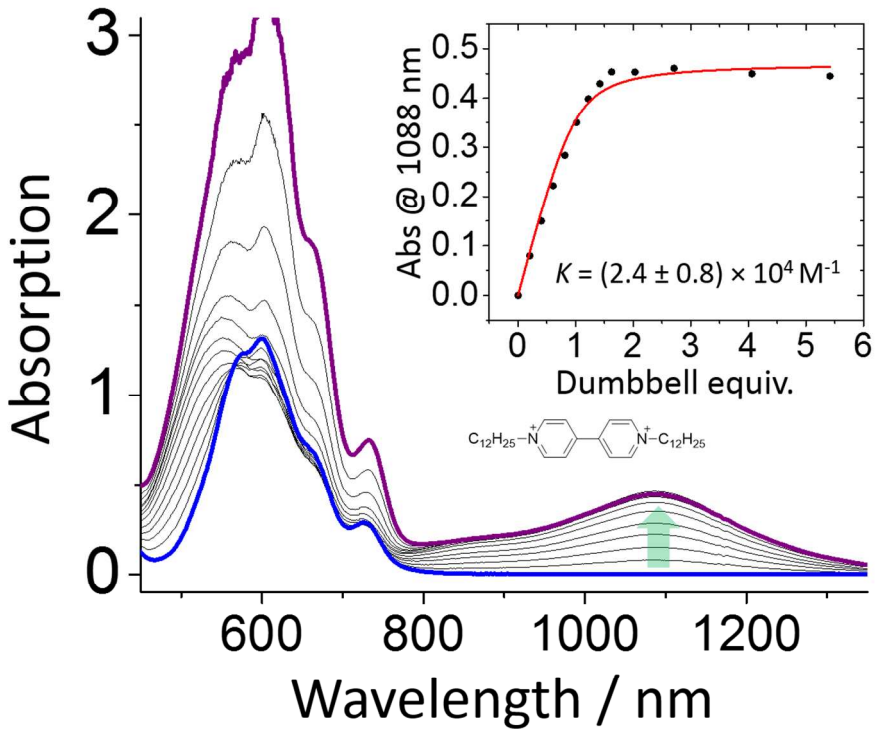


Figure S1 Vis/NIR Spectra of titrating $DB1^{\bullet+}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1088 nm with titration. Curve fitting highlighted in red.

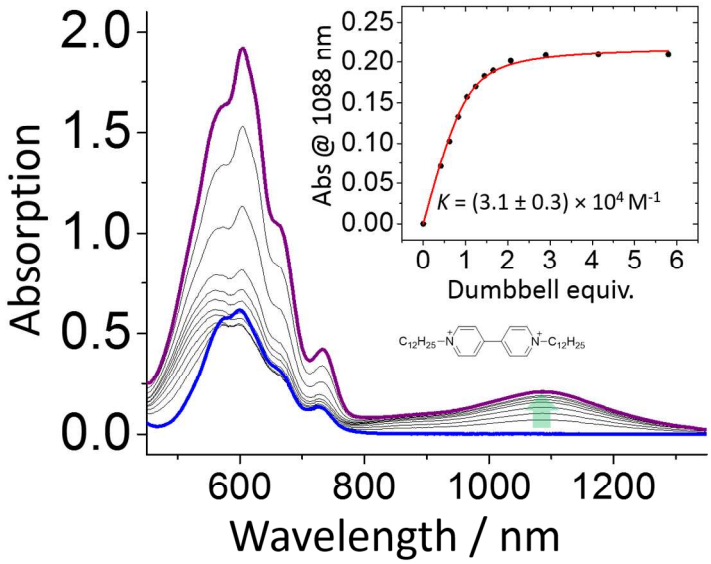


Figure S2 Vis/NIR Spectra of titrating $DB1^{\bullet+}$ into $CBPQT^{2(\bullet+)}$ at a dilute (c_{CBPQT} = 2.5 × 10^{-4} M) condition to reduce the fitting error. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1088 nm with titration. Curve fitting is highlighted in red.

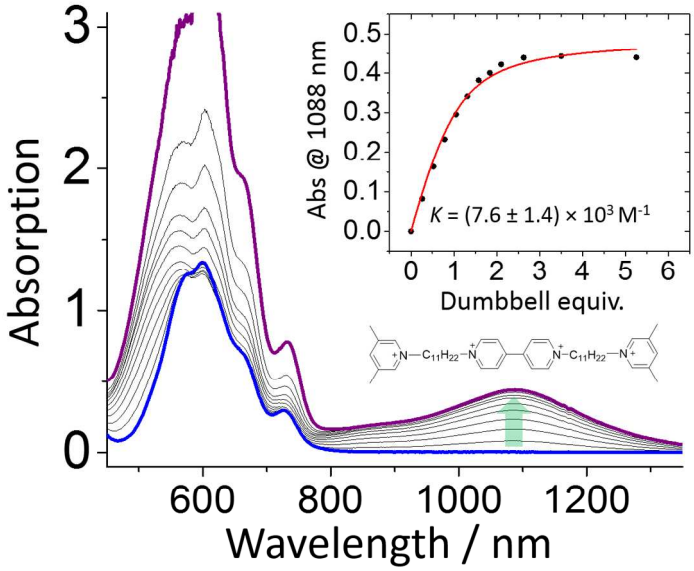


Figure S3 Vis/NIR Spectra of titrating $DB2^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1088 nm with titration. Curve fitting is highlighted in red.

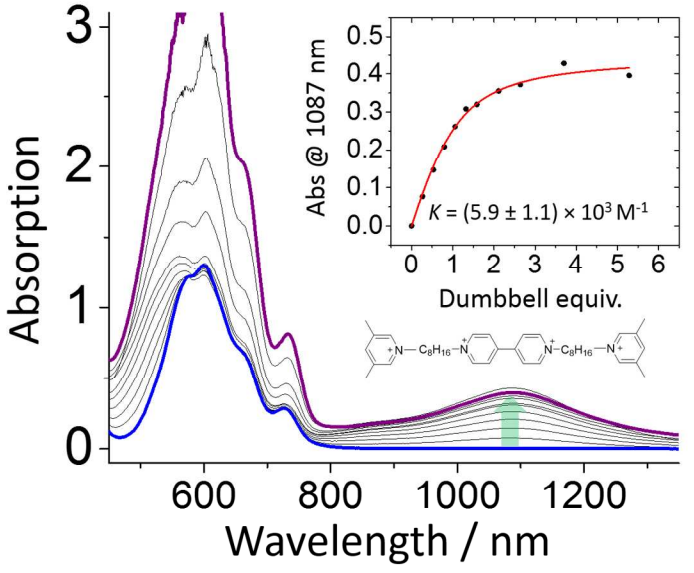


Figure S4 Vis/NIR Spectra of titrating $DB3^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1087 nm with titration. Curve fitting is highlighted in red.

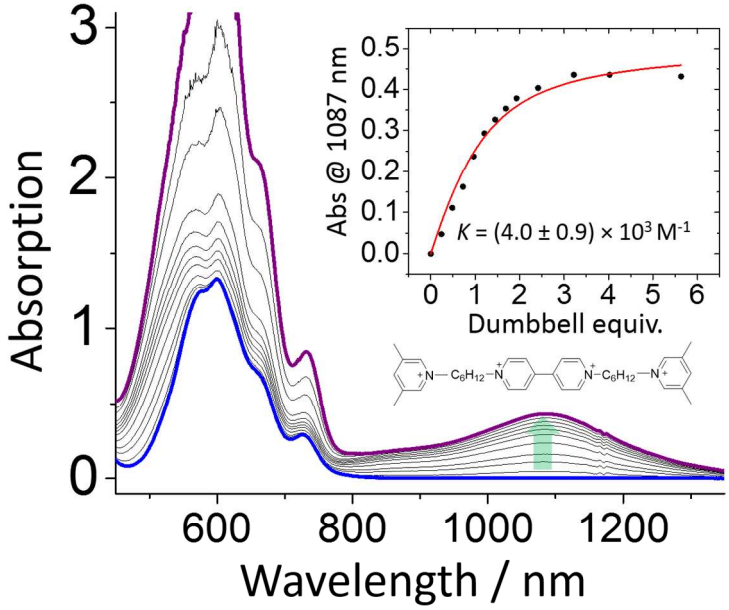


Figure S5 Vis/NIR Spectra of titrating $DB4^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1087 nm with titration. Curve fitting is highlighted in red.

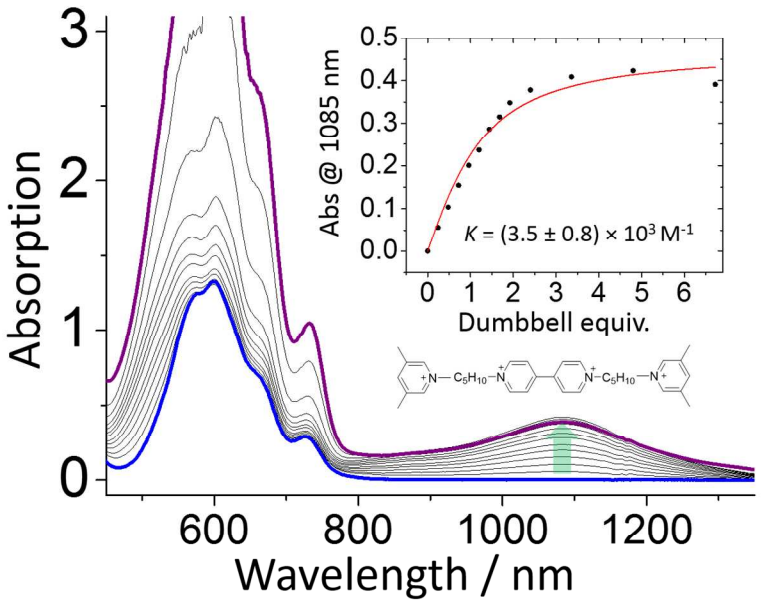


Figure S6 Vis/NIR Spectra of titrating $DB5^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1085 nm with titration. Curve fitting is highlighted in red.

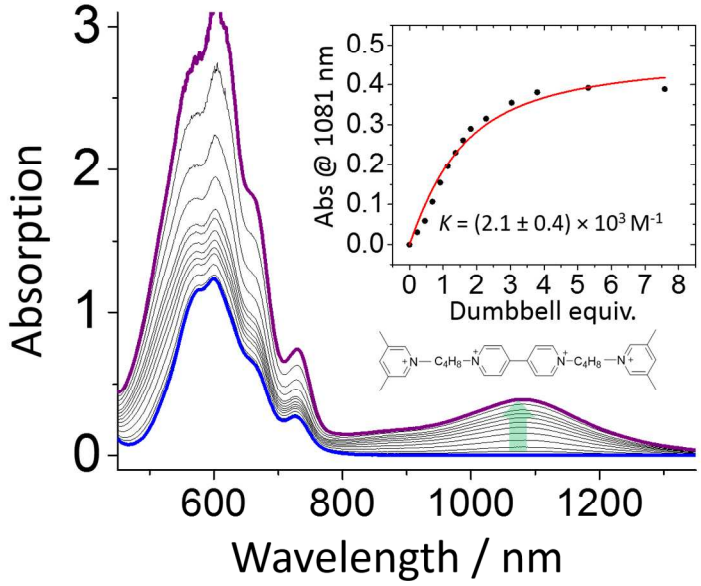


Figure S7 Vis/NIR Spectra of titrating $DB6^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1081 nm with titration. Curve fitting is highlighted in red.

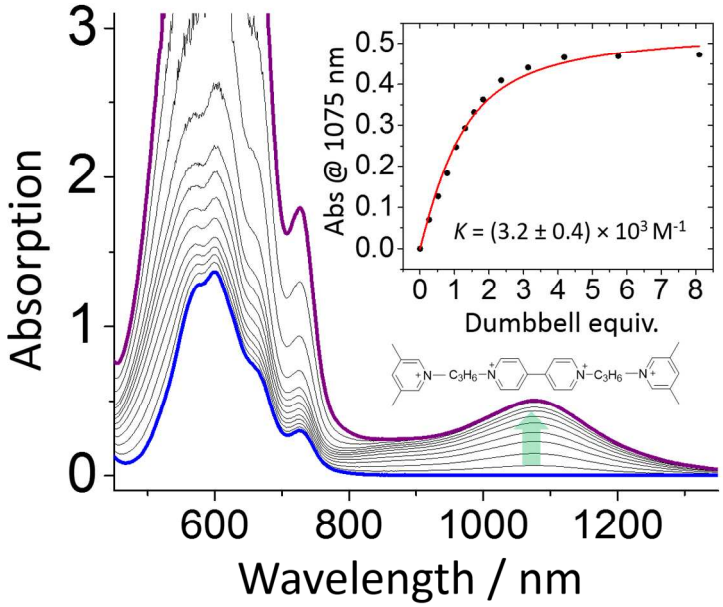


Figure S8 Vis/NIR Spectra of titrating $DB7^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1075 nm with titration. Curve fitting is highlighted in red.

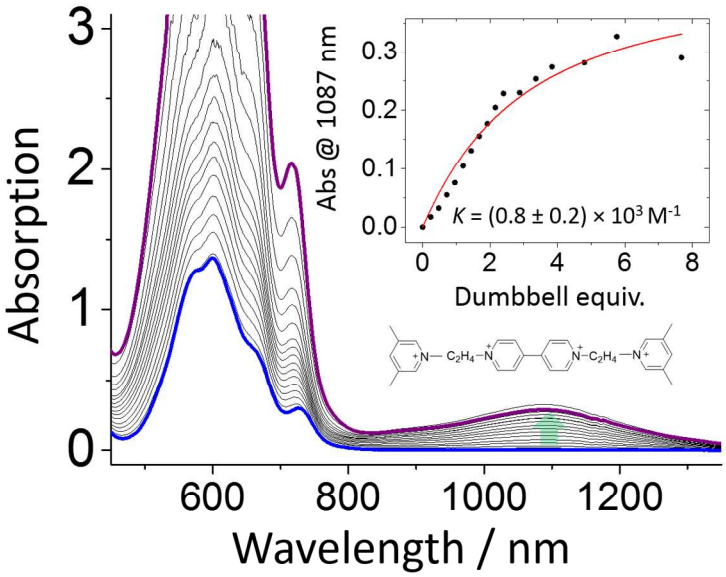


Figure S9 Vis/NIR Spectra of titrating $DB8^{2+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1087 nm with titration. Curve fitting is highlighted in red.

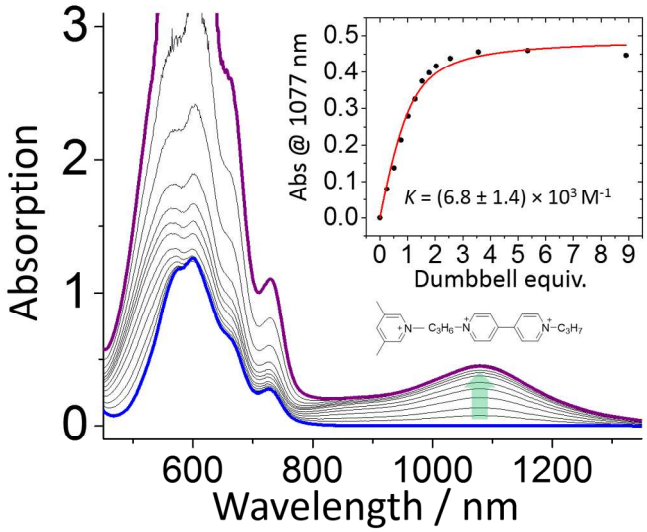


Figure S10 Vis/NIR Spectra of titrating $DB10^{+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1077 nm with titration. Curve fitting is highlighted in red.

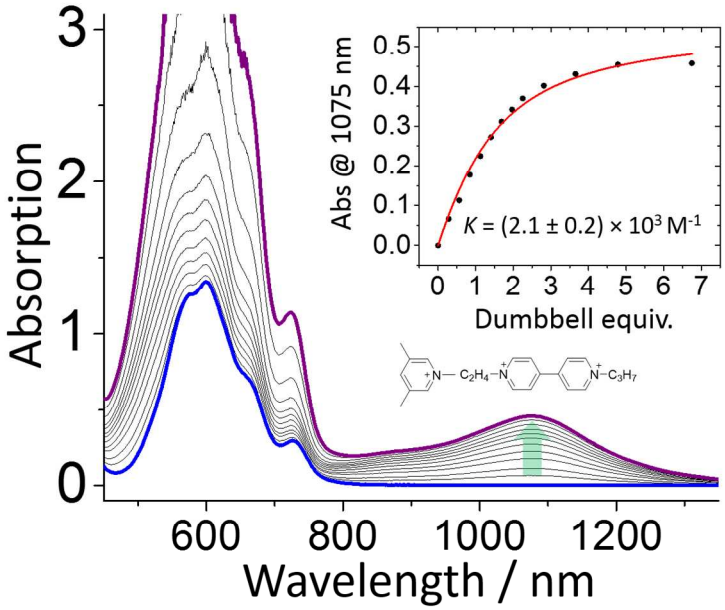


Figure S11 Vis/NIR Spectra of titrating $DB9^{+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1075 nm with titration. Curve fitting is highlighted in red.

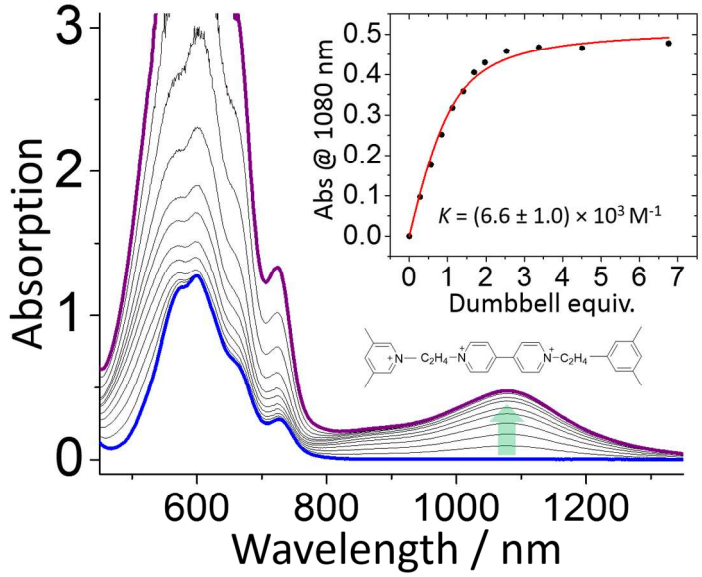


Figure S12 Vis/NIR Spectra of titrating $DB11^{+(\bullet+)}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1080 nm with titration. Curve fitting is highlighted in red.

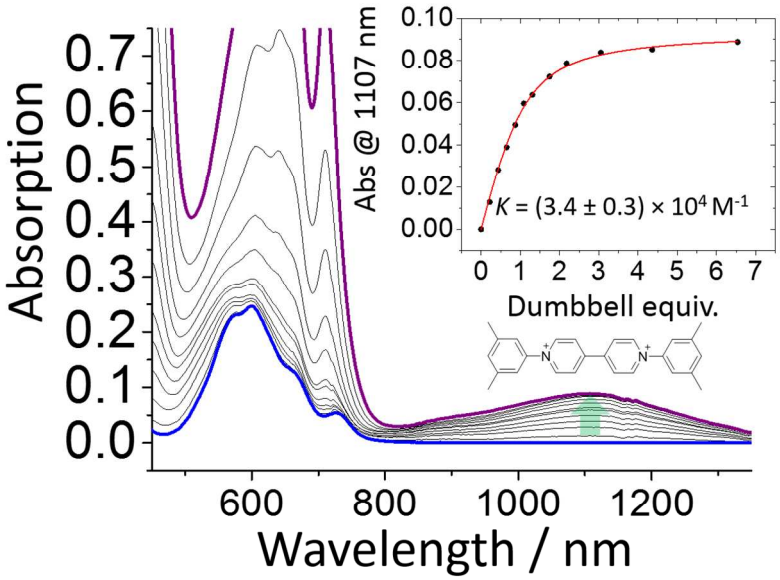


Figure S13 Vis/NIR Spectra of titrating $DB12^{\bullet+}$ into $CBPQT^{2(\bullet+)}$(c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1107 nm with titration. Curve fitting is highlighted in red.

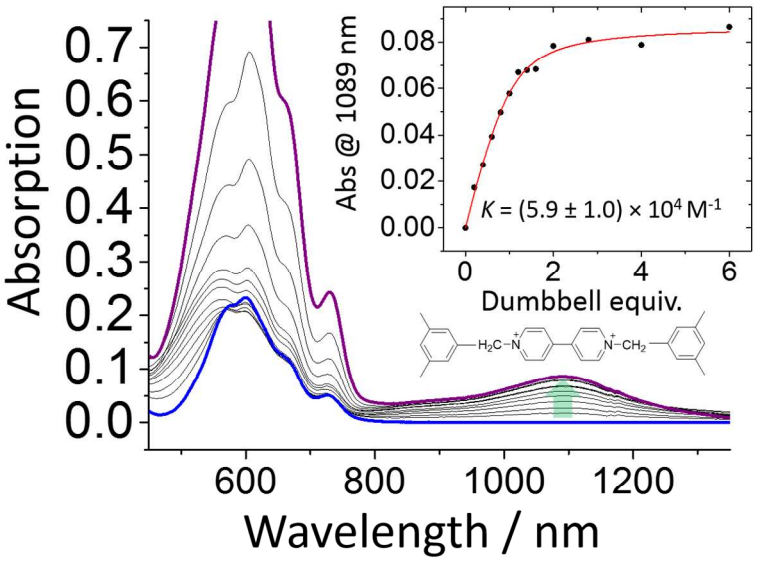


Figure S14 Vis/NIR Spectra of titrating $DB13^{\bullet+}$ into $CBPQT^{2(\bullet+)}$ (c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1089 nm with titration. Curve fitting is highlighted in red.

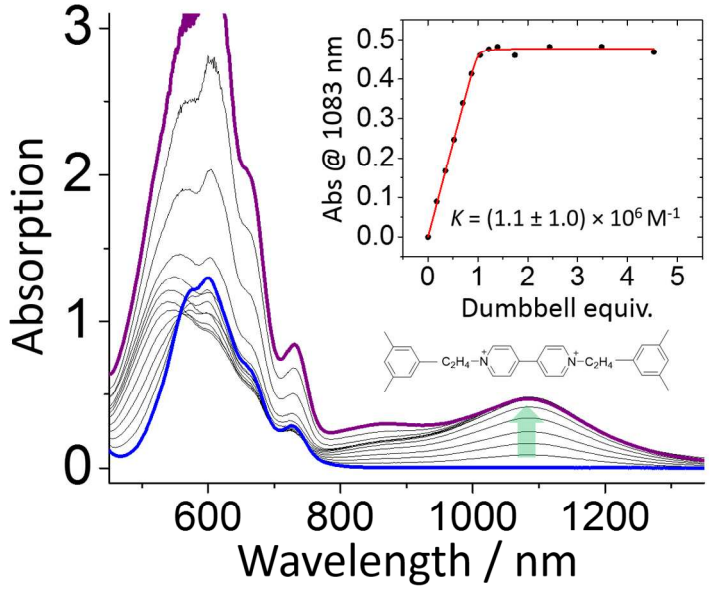


Figure S15 Vis/NIR Spectra of titrating $DB14^{\bullet+}$ into $CBPQT^{2(\bullet+)}$. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1083 nm with titration. Curve fitting is highlighted in red.

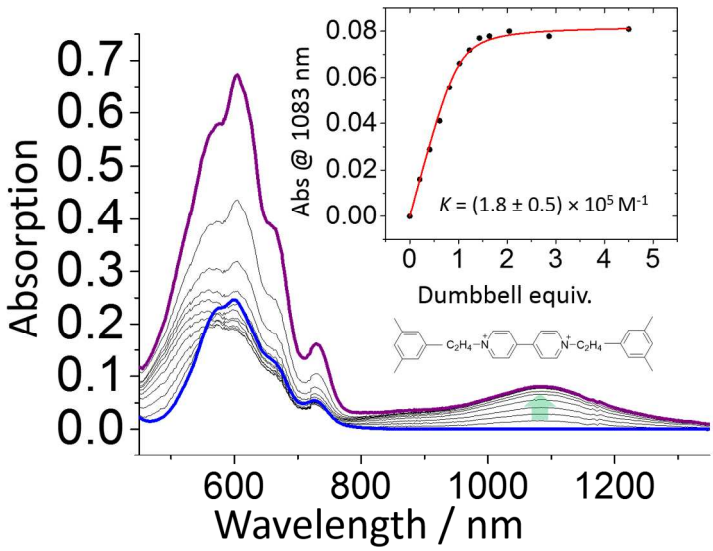


Figure S16 Vis/NIR Spectra of titrating DB14$^{\bullet+}$ into CBPQT$^{2(\bullet+)}$ at a dilute (c_{CBPQT} = 1.0 × 10^{-4} M) condition to reduce fit error. Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1083 nm with titration. Curve fitting is highlighted in red.

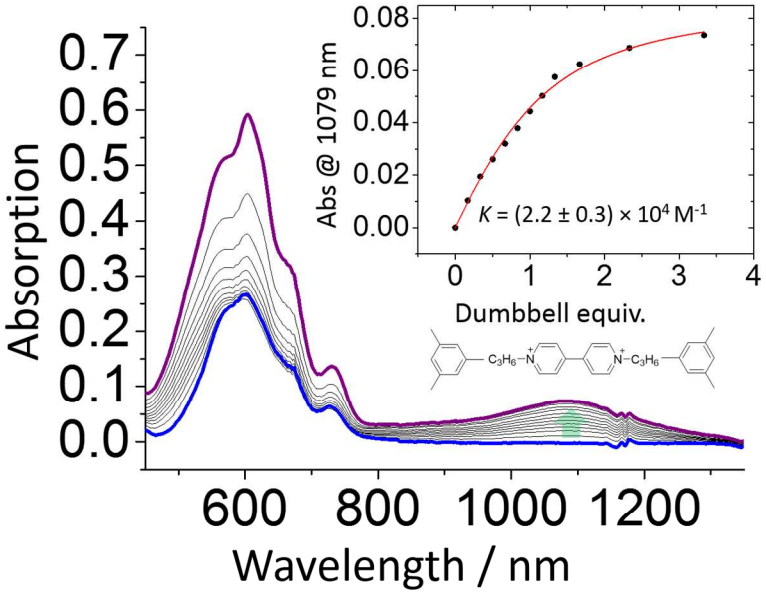


Figure S17 Vis/NIR Spectra of titrating DB15$^{\bullet+}$ into CBPQT$^{2(\bullet+)}$ (c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1079 nm with titration. Curve fitting is highlighted in red.

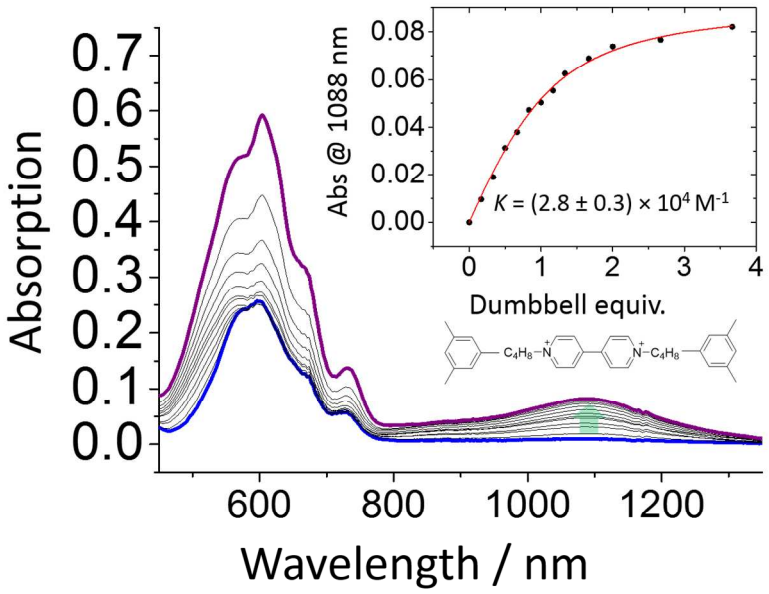


Figure S18 Vis/NIR Spectra of titrating DB16$^{\bullet+}$ into CBPQT$^{2(\bullet+)}$ (c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1088 nm with titration. Curve fitting is highlighted in red.

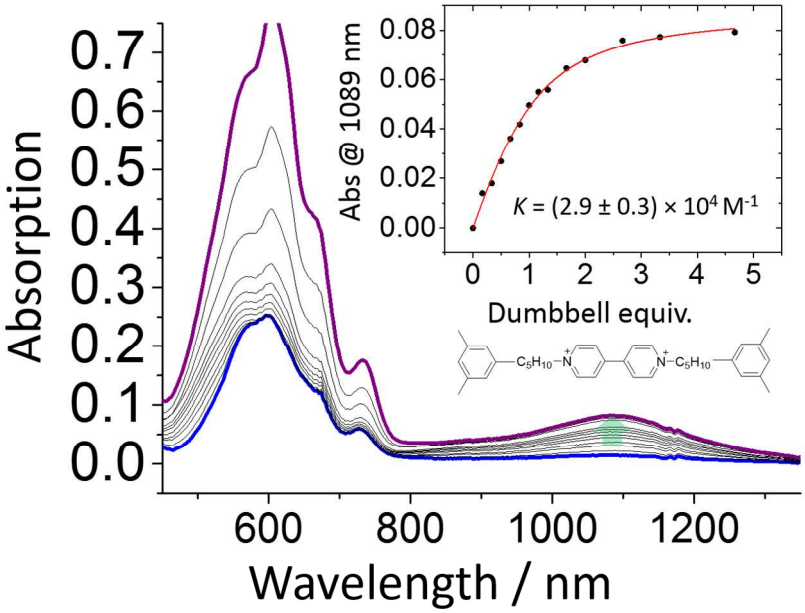


Figure S19 Vis/NIR Spectra of titrating DB17$^{\bullet+}$ into CBPQT$^{2(\bullet+)}$ (c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1086 nm with titration. Curve fitting is highlighted in red.

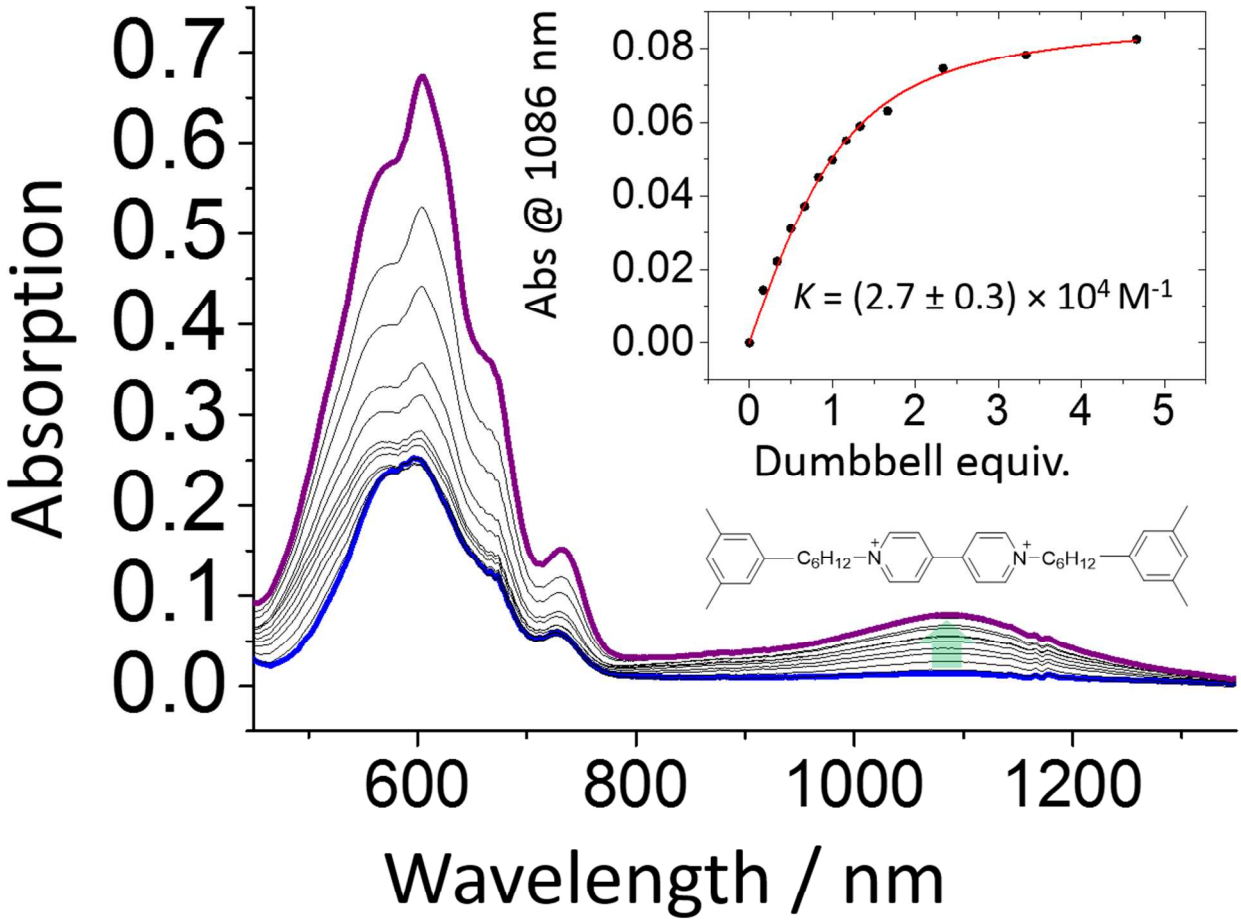
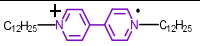
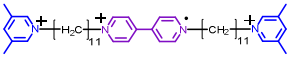
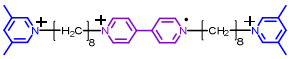
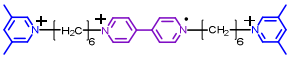
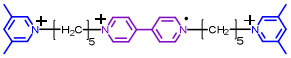
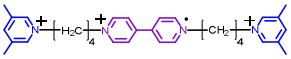
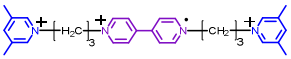
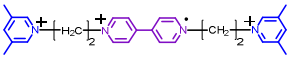
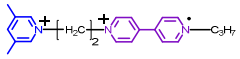
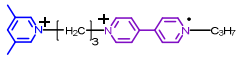
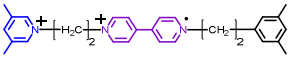
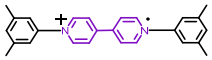
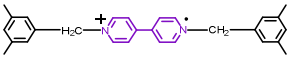
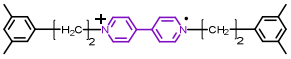
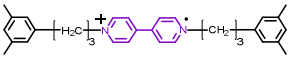
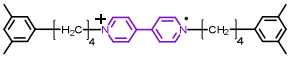
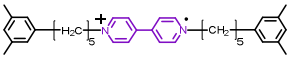
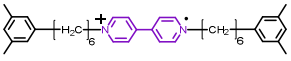


Figure S20 Vis/NIR Spectra of titrating $DB18^{\bullet+}$ into $CBPQT^{2(\bullet+)}$ (c_{CBPQT} = 1.0 × 10^{-4} M). Initial and final spectra are highlighted in blue and purple, respectively. The inset shows the change in absorption at 1086 nm with titration. Curve fitting is highlighted in red.

Table S1. Summary of Binding Constant Measurements

$V^{\bullet+}\subset CBPQT^{2(\bullet+)}$	Dumbbell Structural Formulas	Trisradical Band λ / nm	Binding Constant K / 10^3 M^{-1}	Molar Extinction Coefficient ε / M^{-1} cm^{-1}
$DB1^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1088	31 ± 3	960 ± 40
$DB2^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1088	7.6 ± 1.4	980 ± 40
$DB3^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1087	5.9 ± 1.1	900 ± 40
$DB4^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1087	4.0 ± 0.9	1020 ± 60
$DB5^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1085	3.5 ± 0.8	940 ± 60
$DB6^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1081	2.5 ± 0.4	960 ± 60
$DB7^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1075	3.2 ± 0.4	1080 ± 40
$DB8^{2+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1087	0.8 ± 0.1	880 ± 60
$DB9^{+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1075	2.1 ± 0.2	1120 ± 40
$DB10^{+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1077	6.8 ± 1.4	980 ± 40
$DB11^{+(\bullet+)}\subset CBPQT^{2(\bullet+)}$		1080	6.6 ± 1.0	1040 ± 20
$DB12^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1107	34 ± 3	940 ± 10
$DB13^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1089	59 ± 10	870 ± 20
$DB14^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1083	177 ± 46	820 ± 20
$DB15^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1079	22 ± 3	890 ± 30
$DB16^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1088	28 ± 3	930 ± 20
$DB17^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1086	27 ± 3	890 ± 20
$DB18^{\bullet+}\subset CBPQT^{2(\bullet+)}$		1087	29 ± 3	900 ± 20

4. Single Crystal X-Ray Diffraction

General Procedures for Growing Single Crystals: Excess of activated Zn dust was added to a mixture of CBPQT•4PF_6 (0.6 mg, 0.5 μmol) and the dumbbells (0.5 μmol, DB8•4PF_6, DB9•4PF_6, DB10•4PF_6, DB12•2PF_6, DB13•2PF_6, or DB14•2PF_6) in MeCN (1 mL) in a glovebox, and the mixtures were stirred for 30 min. After filtering, the purple solutions were kept under an atmosphere of iPr_2O at 0 °C to allow slow vapor diffusion to occur.

The single crystal XRD of DB7⊂CBPQT•6PF_6 (**Figure S21**) is reported in our previous report.[3]

DB8⊂CBPQT•5PF_6 (**Figure S22**): Single crystals suitable for X-ray diffraction were mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector equipped with a CuKα microsource with MX optics. SADABS-2012/1 (Bruker,2012) was used for absorption correction. *wR*2(int) was 0.1116 before and 0.0653 after correction. The ratio of minimum to maximum transmission is 0.7784. The $\lambda/2$ correction factor is 0.0015.

Crystal Data for $C_{72}H_{78}F_{30}N_{12}P_5$, M =1836.34, triclinic, space group $P\bar{1}$ (no. 2), a = 13.9238(14), b = 18.0258(17), c = 19.2008(18) Å, α = 87.542(5), β = 74.700(6), γ = 83.934(6)°, V = 4621.8(8) $Å^3$, Z = 2, T = 99.99, μ(CuKα) = 1.858, 31230 reflections measured, 14749 unique (R_{int} = 0.0624) which were used in all calculations. The final $wR(F_2)$ was 0.5072 (all data). Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476153.

Refinement Details. Five PF_6^- anions were restrained in six sites. Distance restraints were used for the PF_6^- anions. Rigid bond restraints were imposed on the displacement parameters as well as restraints on similar amplitudes separated by less than 1.7 Å. on disordered atoms. Group displacement parameters were refined for the disordered five PF_6^- anions.

Solvent Treatment Details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula. Total solvent accessible volume / cell = 488.2 $Å^3$ [10.6%] Total electron count / cell = 34.8.

DB9⊂CBPQT•4PF_6 (**Figure S23**): A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector diffractometer. The crystal was kept at 100 K during data collection. Using Olex2[6], the structure was solved with the XM[7] structure solution program using Dual Space and refined with the XL[7] refinement package using Least Squares minimization.

Crystal Data for $C_{59}H_{62}F_{24}N_7P_4$, M =1449.03, triclinic, space group $P\bar{1}$ (no. 2), a = 16.640(4), b = 16.710(3), c = 17.160(4) Å, α = 75.037(13), β = 70.814(13), γ = 62.956(14)°, V = 3979.9(16) Å^3, Z = 2, T = 100.02 K, μ(CuKα) = 1.710 mm^{-1}, D_{calc} = 1.209 g/mm^3, 12511 reflections measured ($5.498 \leq 2\Theta \leq 108.322$), 8609 unique ($R_{int}$ = 0.0596, R_{sigma} = 0.1371) which were used in all calculations. The final R_1 was 0.1078 ($I > 2\sigma(I)$) and wR_2 was 0.3129 (all data). Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476154.

Refinement Details. The enhanced rigid bond restraint (RIGU) was applied globally. Other restraints on displacement parameters (DELU, SIMU, ISOR) were applied to the C, N atoms of the CBPQT ring as well as disordered C atoms.

Solvent Treatment Details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 1117.1 Å^3 [28.1%] Total electron count / cell = 151.4.

DB10⊂CBPQT•4PF_6 (**Figure S24**): A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa Apex2 diffractometer. The crystal was kept at 100(2) K during data collection. Using Olex2[6], the structure was solved with the XM[7] structure solution program using Dual Space and refined with the ShelXL[7] refinement package using Least Squares minimization.

Crystal Data for $C_{61}H_{64.5}F_{24}N_{8.5}P_4$, M =1496.59, triclinic, space group $P\bar{1}$ (no. 2), a = 13.8924(9), b = 19.3041(11), c = 28.5592(17) Å, α = 87.962(4), β = 83.733(4), γ = 75.084(4)°, V = 7356.5(8) Å^3, Z = 4, T = 100(2) K, μ(CuKα) = 1.874 mm^{-1}, D_{calc} = 1.351 g/mm^3, 14372 reflections measured ($3.112 \leq 2\Theta \leq 101.114$), 14372 unique ($R_{sigma}$ = 0.1201) which were used in all calculations. The final R_1 was 0.1187 ($I > 2\sigma(I)$) and wR_2 was 0.3391 (all data).

Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476155.

Refinement Details. The crystal used for this experiment was non-merohedrally twinned. The twin law, identified by the program Cell Now was found to be a 180° rotation about the reciprocal *c*-axis. The final twin matrix was determined with the integration program SAINT to be (−0.99945 −0.00144 −0.00016 / 0.00263 −1.00052 0.00073 /−0.44152 −0.02214 0.99997). The absorption correction was carried out using TWINABS to create an HKLF4 file which was used to solve the structure, and an HKLF5 file which was used for refinements. The twin fraction refined to a value of 0.1582(15).

Solvent Treatment Details. The program SQUEEZE (Platon) was used to provide a fixed solvent contribution to F_{calc} to use in refinement against F_{obs}.

DB12⊂CBPQT•3PF_6 (**Figure S25**) A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector diffractometer. The crystal was kept at 99.99 K during data collection. Using Olex2[6], the structure was solved with the XM[7] structure solution program using Dual Space and refined with the XL[7] refinement package using Least Squares minimization.

Crystal Data for $C_{64}H_{61}F_{18}N_7P_3$ (M =1363.10): monoclinic, space group $C2/m$ (no. 12), a = 27.8633(18), b = 19.6876(13), c = 14.3635(9) Å, β = 121.019(2)°, V = 6752.5(8) Å^3, Z = 4, T = 99.99 K, μ(CuKα) = 1.635 mm^{-1}, *Dcalc* = 1.341 g/mm^3, 23953 reflections measured (7.182 ≤ 2Θ ≤ 130.168), 5897 unique (R_{int} = 0.0279, R_{sigma} = 0.0237) which were used in all calculations. The final R_1 was 0.1005 ($I > 2\sigma(I)$) and wR_2 was 0.3082 (all data). Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476156.

Refinement Details. Chemically equivalent P–F and F–F distances for the disordered PF_6^- anion were refined with similarity restraints (SADI).

Solvent Treatment Details. The solvent masking procedure as implemented in Olex2 was used to remove the electronic contribution of solvent molecules from the refinement. As the exact solvent content is not known, only the atoms used in the refinement model are reported in the formula here. Total solvent accessible volume / cell = 860.5 Å^3 [12.7%] Total electron count / cell = 174.1

DB13⊂CBPQT•3.5PF_6 (**Figure S26**) A suitable crystal was selected and mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector diffractometer. The crystal was kept at 99.99 K during data collection. Using Olex2[6], the structure was solved with the XM[7] structure solution program using Dual Space and refined with the XL[7] refinement package using Least Squares minimization.

Crystal Data for $C_{146}H_{151}F_{42}N_{21}P_7$ (M =3214.66): monoclinic, space group $P2_1/n$ (no. 14), a = 16.6492(7), b = 19.7296(9), c = 22.6647(10) Å, β = 95.147(3)°, V = 7414.9(6) Å^3, Z = 2, T = 99.99 K, μ(CuKα) = 1.751 mm^{-1}, *Dcalc* = 1.440 g/mm^3, 35068 reflections measured (5.95 ≤ 2Θ ≤ 130.378), 12522 unique (R_{int} = 0.0514, R_{sigma} = 0.0529) which were used in all calculations. The final R_1 was 0.0582 (I > 2σ(I)) and wR_2 was 0.1747 (all data). Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476157.

Refinement Details. Chemically equivalent distances in the disordered MeCN solvent molecules and for the disordered PF_6^- anion position, were refined with similarity restraints (SADI). The enhanced rigid-bond restraint (RIGU) was applied globally. The occupancies of the PF_6^- anion disordered with MeCN were refined freely to approximately 50%. We believe the approximately 50% occupancies of PF_6^- anion indicates this structure contains cations in both the 3+ and 4+ oxidation states and consequently there are 7 PF_6^- anions for two molecules.

DB14⊂CBPQT•3PF_6 (**Figure S27**): A single crystal suitable for X-ray diffraction was mounted in inert oil and transferred to the cold gas stream of a Bruker Kappa APEX CCD area detector equipped with a CuKα microsource with MX optics. SADABS-2012/1 (Bruker,2012) was used for absorption correction. wR_2(int) was 0.0768 before and 0.0456 after correction. The ratio of minimum to maximum transmission is 0.8720. The λ/2 correction factor is 0.0015.

Crystal Data for $C_{70}H_{72}F_{18}N_8P_3$, M =1460.26, triclinic, space group $P\bar{1}$ (no. 2), a = 9.938(2), b = 13.616(3), c = 14.482(3) Å, α = 113.563(6), β = 99.933(7), γ = 101.953(7)°, V = 1684.5(6) Å^3, Z = 1, T = 99.99, μ(CuKα) = 1.682, 31989 reflections measured, 6073 unique (R_{int} = 0.0257) which were used in all calculations. The final $wR(F_2)$ was 0.0824 (all data). Crystallographic data (excluding structure factors) for the structures reported in this article have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC–1476158.

Refinement Details. No special restraints or constraints were used in this refinement. All hydrogen atoms were located from residual density maps and freely refined.

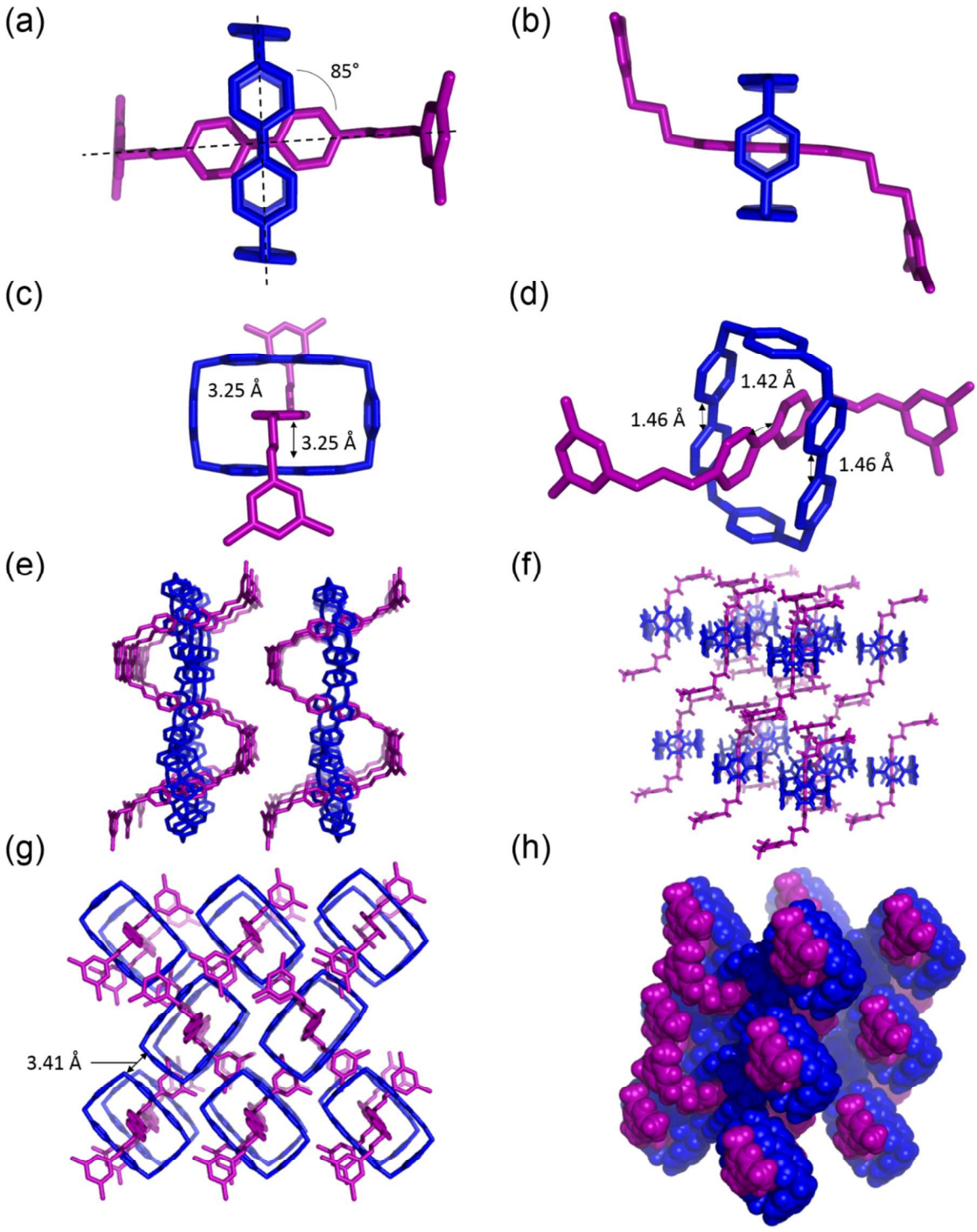


Figure S21. Solid-state superstructures of DB7⊂CBPQT•6PF_6 (a) and (b) side-on views, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB7⊂CBPQT•6PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

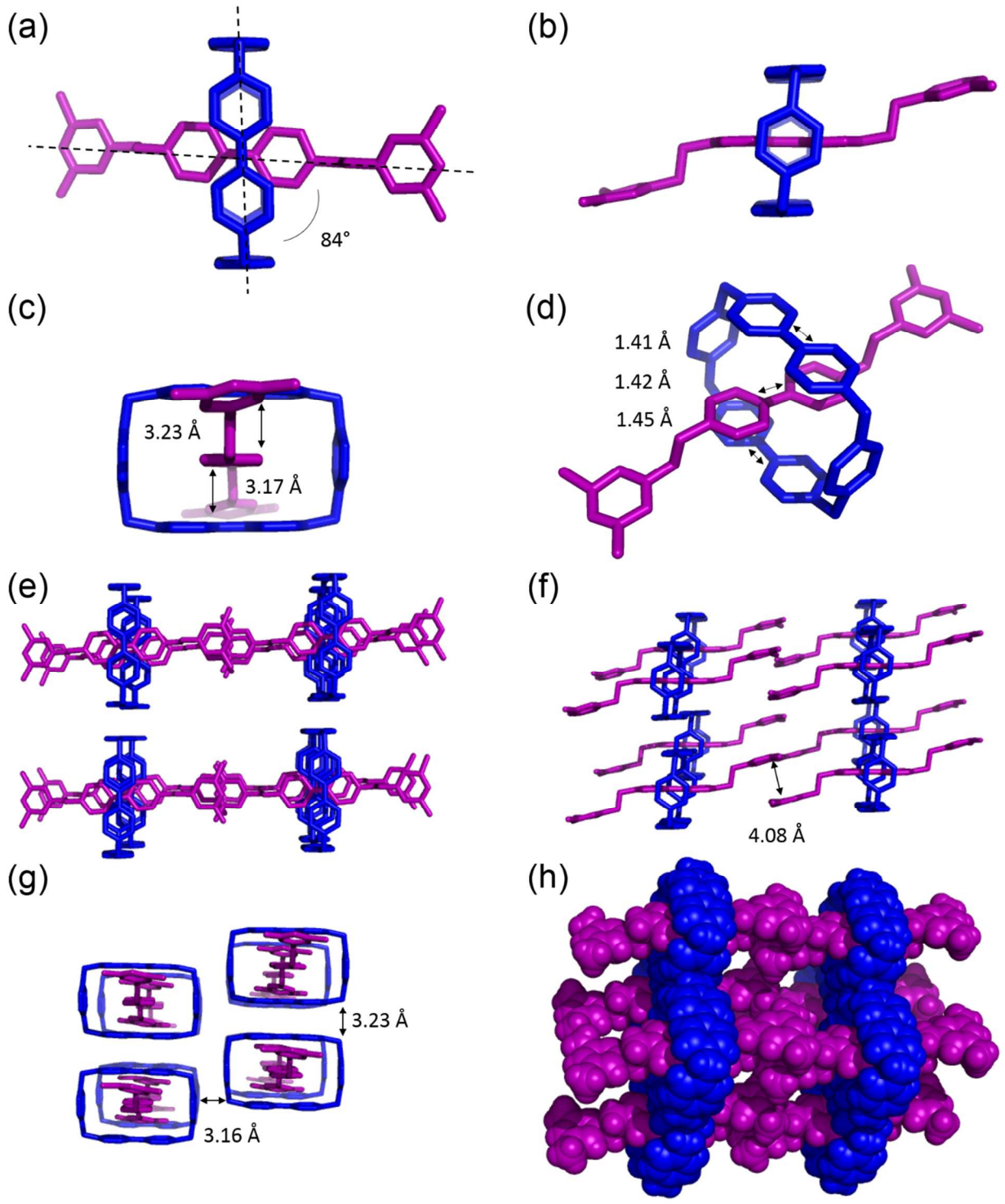


Figure S22. Solid-state superstructures of DB8⊂CBPQT•5PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB8⊂CBPQT•5PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

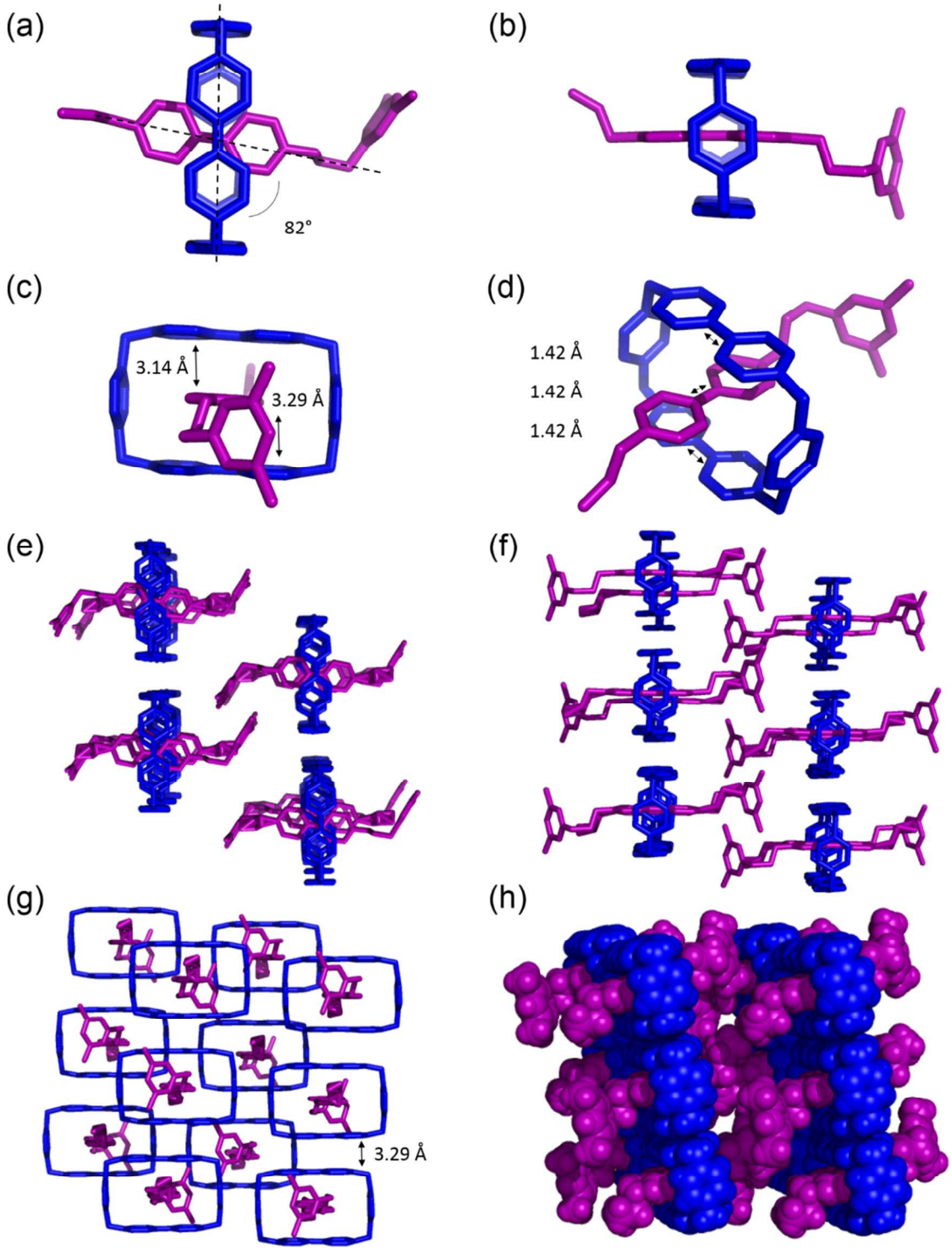


Figure S23. Solid-state superstructures of DB9⊂CBPQT•4PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB9⊂CBPQT•4PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

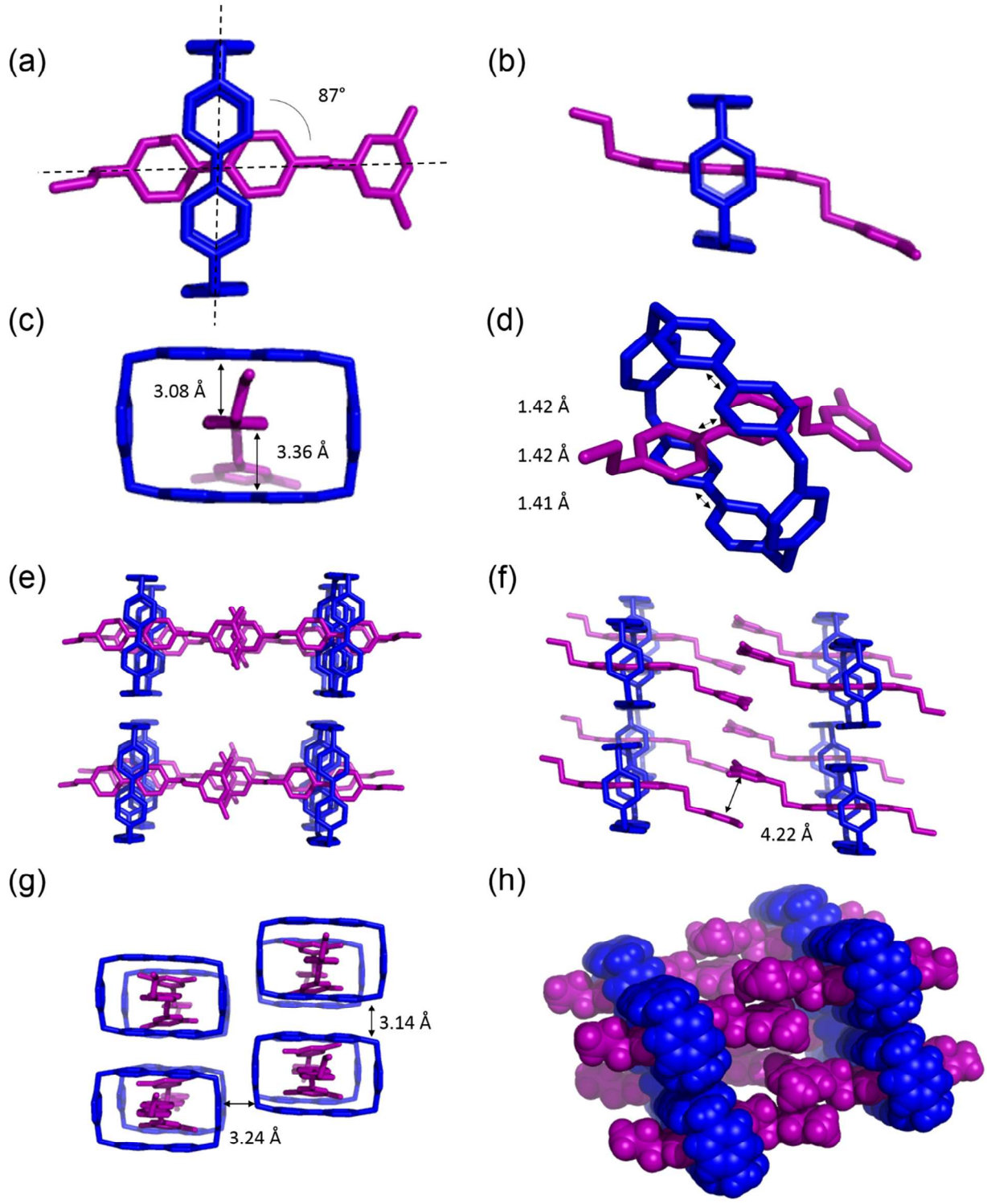


Figure S24. Solid-state superstructures of DB10⊂CBPQT•4PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB10⊂CBPQT•4PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

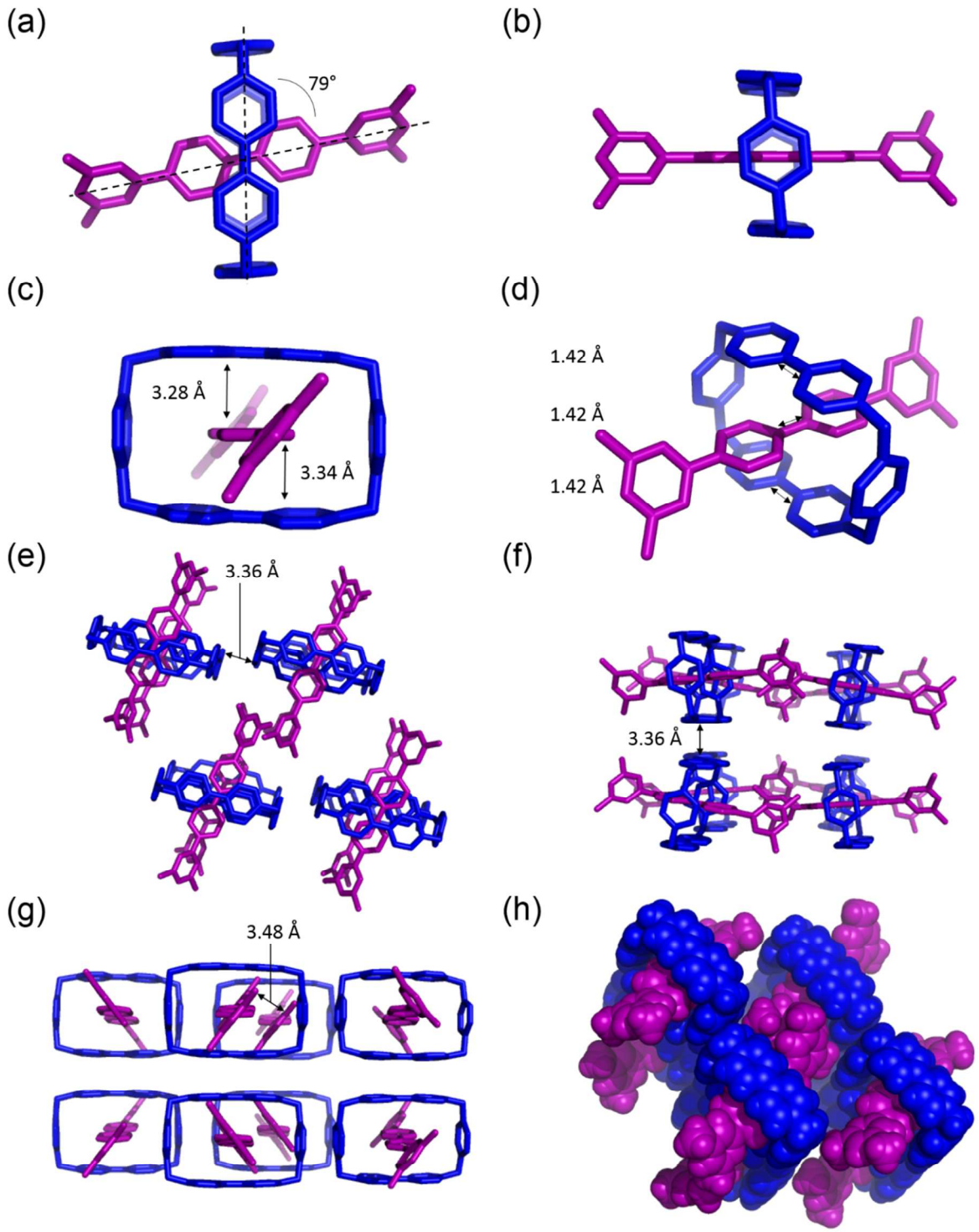


Figure S25. Solid-state superstructures of DB12⊂CBPQT•3PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB12⊂CBPQT•3PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

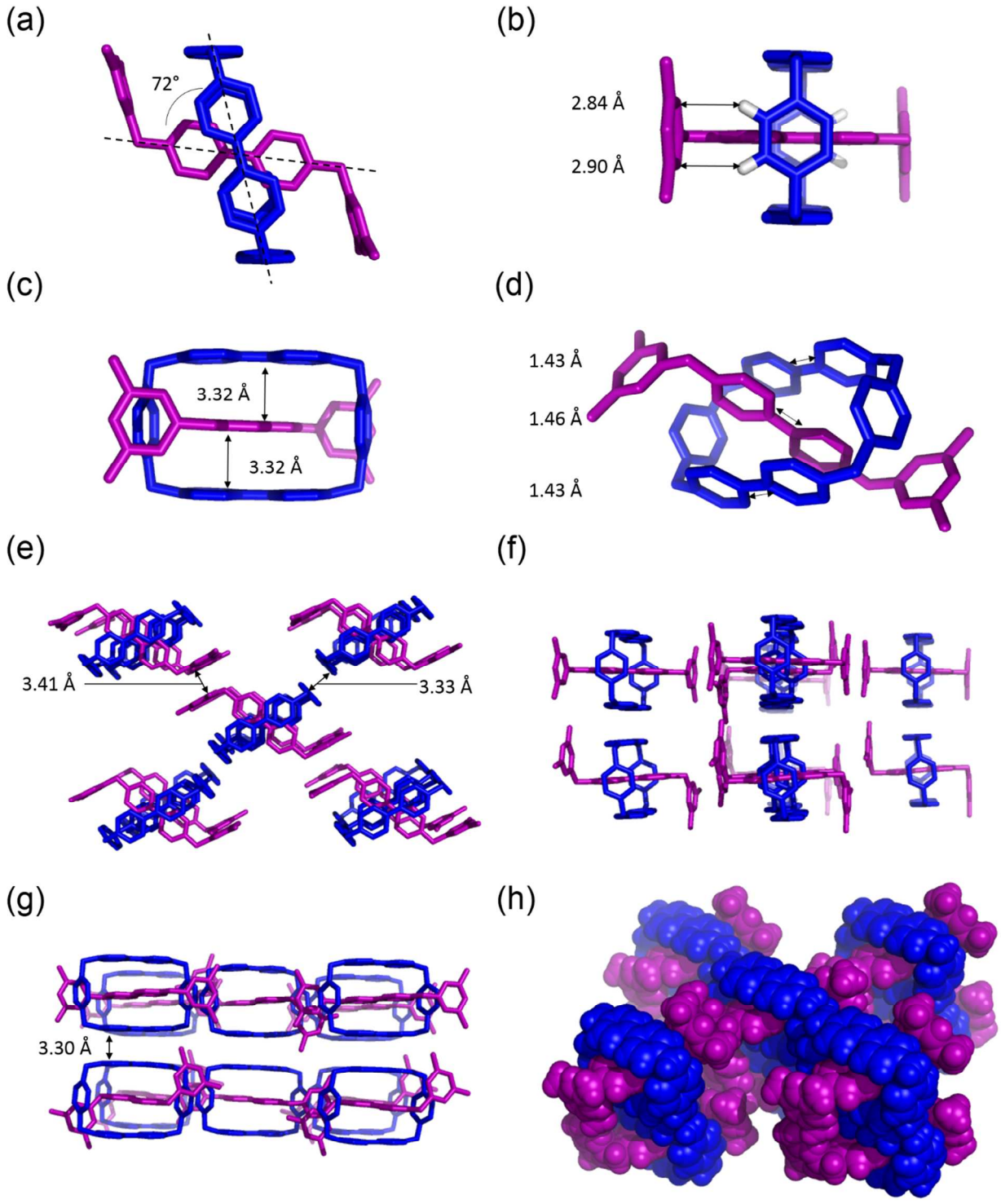


Figure S26. Solid-state superstructures of DB13⊂CBPQT•3.5PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB13⊂CBPQT•3.5PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

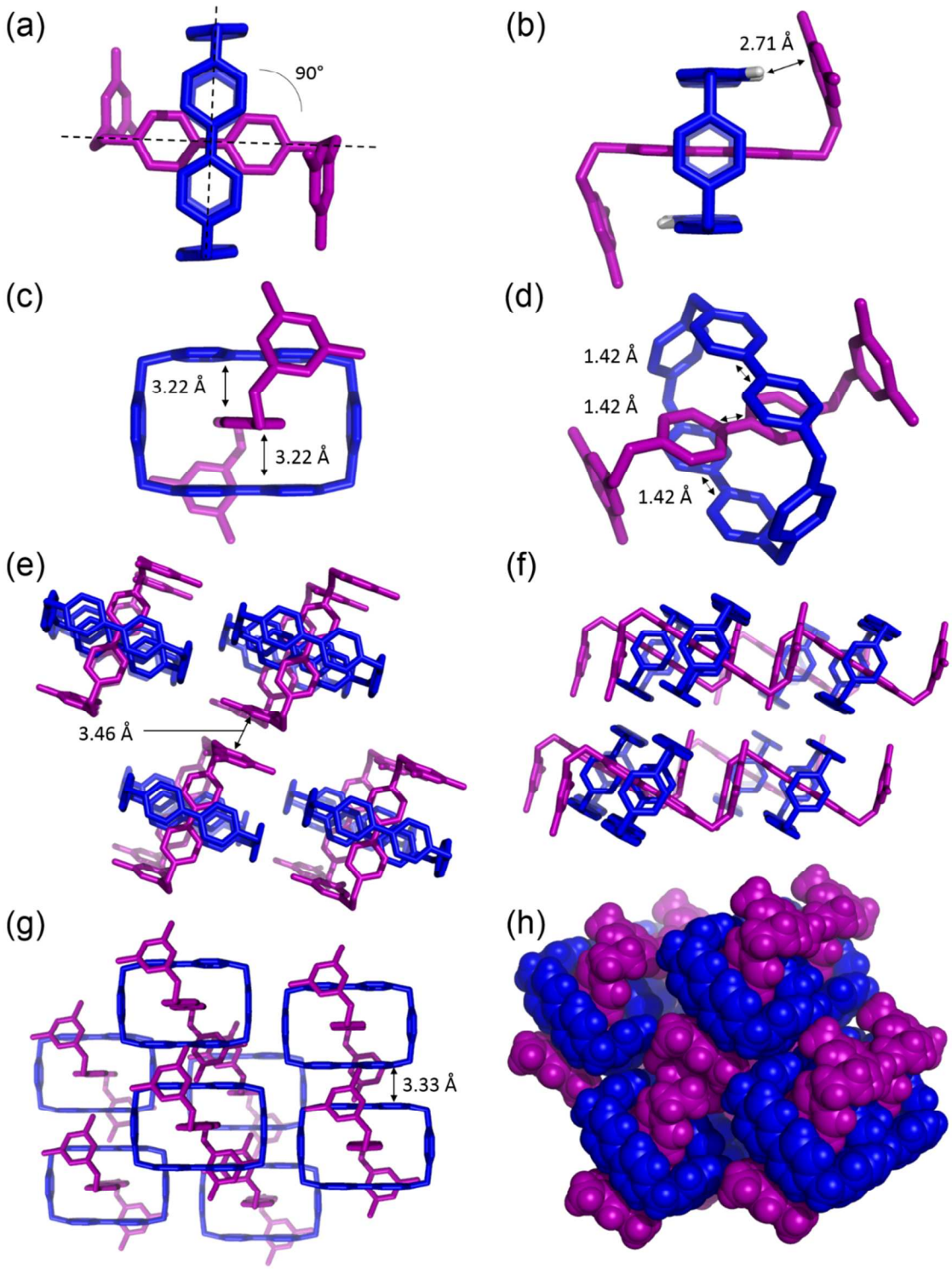


Figure S27. Solid-state superstructures of DB14⊂CBPQT•3PF_6 (a) and (b) side-on view, (c) plan view, (d) perspective view. Solid-state superstructures packing of DB14⊂CBPQT•3PF_6 (e) and (f) side-on view, (g) plan view, (h) space-filling perspective view. Solvent molecules and counterions are omitted for the sake of clarity.

5. Cyclic Voltammetry (CV) Measurements

General Procedures for CV Experiments: Each dumbbell compound (1 mmol) was dissolved in 1 mL MeCN solution (TBA•PF_6, 0.1 M). 0.5 mL of the dumbbell solution was mixed with 0.5 mL MeCN solution (CBPQT•$4PF_6$ 1 mM, TBA•PF_6 0.1 M) to afford 1:1 dumbbell/$CBPQT^{4+}$ samples, and the other 0.5 mL of the dumbbell solution was diluted with 0.5 mL MeCN solution (TBA•PF_6 0.1 M) to afford the dumbbell only sample with an analyte concentration of 0.5 mM. Cyclic voltammograms of dumbbells are compared in **Figure S28–S30** and the data are summarized in **Table S2**. Variable scan rate CV results from 1:1 mixture dumbbell/$CBPQT^{4+}$ samples are shown in **Figure S31**.

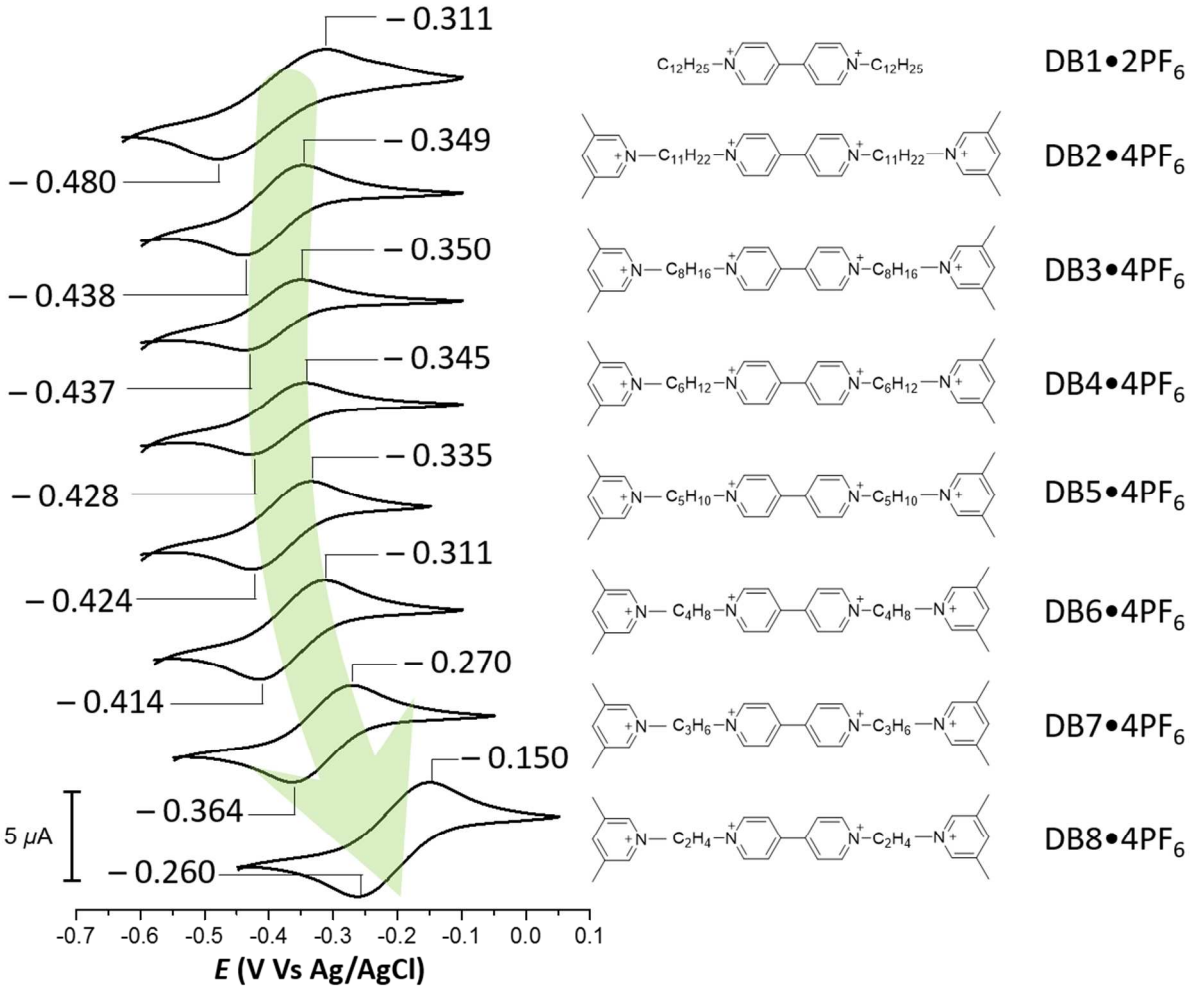


Figure S28. Cyclic voltammograms (0.5 mM in MeCN, 0.1 M $TBAPF_6$, 100 $mV \cdot s^{-1}$, 298 K) of DB1•$2PF_6$, DB2–DB8•$4PF_6$ show the influence on redox potentials from the linker lengths of the charged end groups.

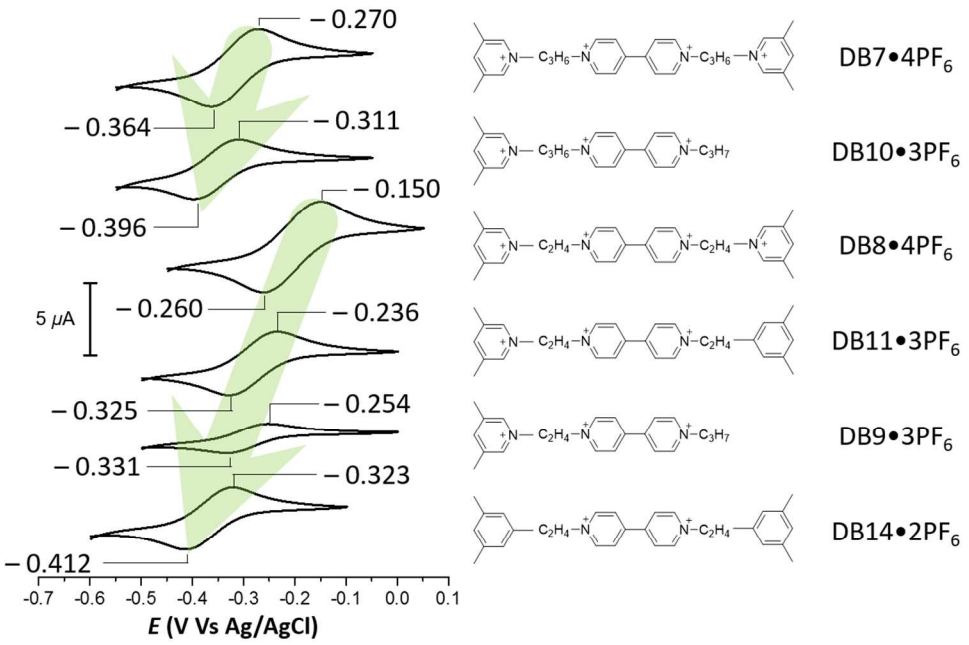


Figure S29. Cyclic voltammograms (0.5 mM in MeCN, 0.1 M $TBAPF_6$, 100 $mV \cdot s^{-1}$, 298 K) of DB7–DB8•$4PF_6$, DB9–DB11•$3PF_6$ and DB14•$2PF_6$ show the influence on redox potentials from the number of the charged end groups.

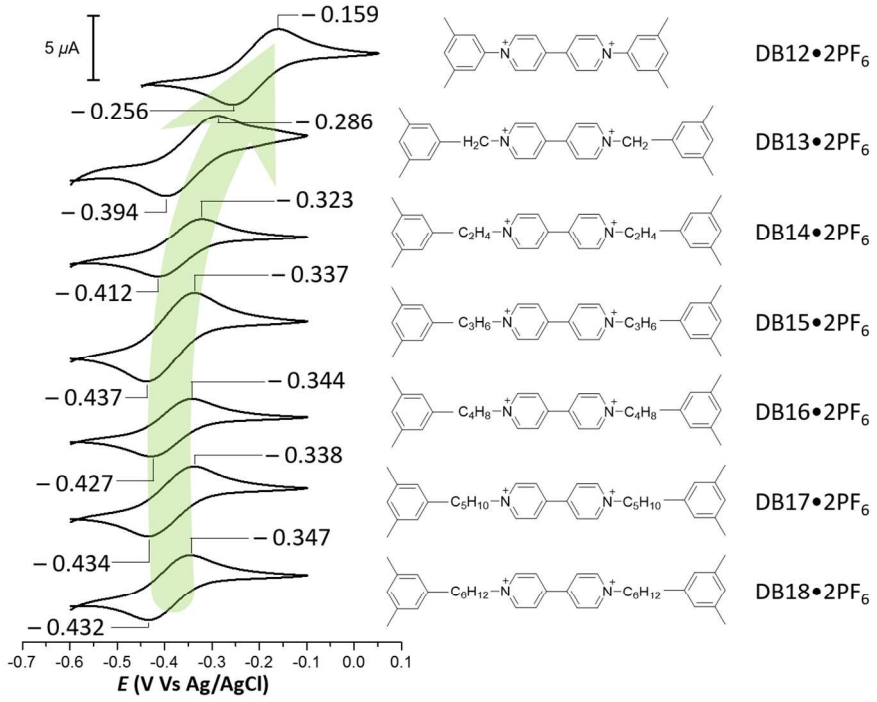
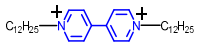
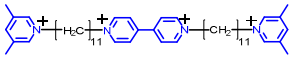
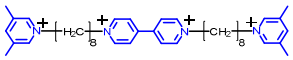
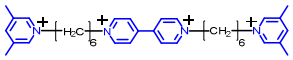
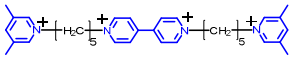
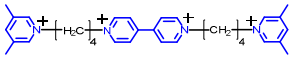
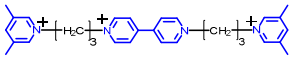
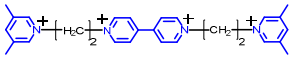
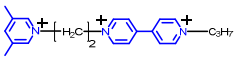
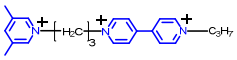
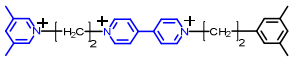
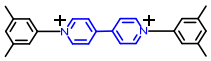
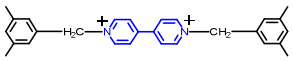
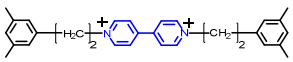
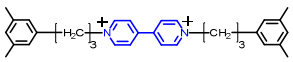
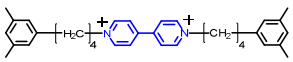
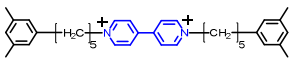
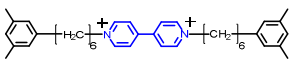


Figure S30. Cyclic voltammograms (0.5 mM in MeCN, 0.1 M $TBAPF_6$, 100 $mV \cdot s^{-1}$, 298 K) of DB12–DB18•$2PF_6$ show the influence on redox potentials from the linker lengths of the neutral end groups.

Table S2. Summary of Cyclic Voltammetry Data of Dumbbells

Dumbbells	Dumbbell Structural Formules	Reduction Peak E / V	Oxidation peak E / V	Average E / V
$DB1^{2+}$		– 0.480	– 0.311	– 0.396
$DB2^{4+}$		– 0.438	– 0.349	– 0.394
$DB3^{4+}$		– 0.437	– 0.350	– 0.394
$DB4^{4+}$		– 0.428	– 0.345	– 0.386
$DB5^{4+}$		– 0.424	– 0.335	– 0.380
$DB6^{4+}$		– 0.414	– 0.311	– 0.362
$DB7^{4+}$		– 0.364	– 0.270	– 0.317
$DB8^{4+}$		– 0.260	– 0.150	– 0.205
$DB9^{3+}$		– 0.331	– 0.254	– 0.292
$DB10^{3+}$		– 0.396	– 0.311	– 0.354
$DB11^{3+}$		– 0.325	– 0.236	– 0.280
$DB12^{2+}$		– 0.256	– 0.159	– 0.208
$DB13^{2+}$		– 0.394	– 0.286	– 0.340
$DB14^{2+}$		– 0.412	– 0.323	– 0.368
$DB15^{2+}$		– 0.437	– 0.337	– 0.387
$DB16^{2+}$		– 0.427	– 0.344	– 0.386
$DB17^{2+}$		– 0.434	– 0.338	– 0.386
$DB18^{2+}$		– 0.432	– 0.347	– 0.390

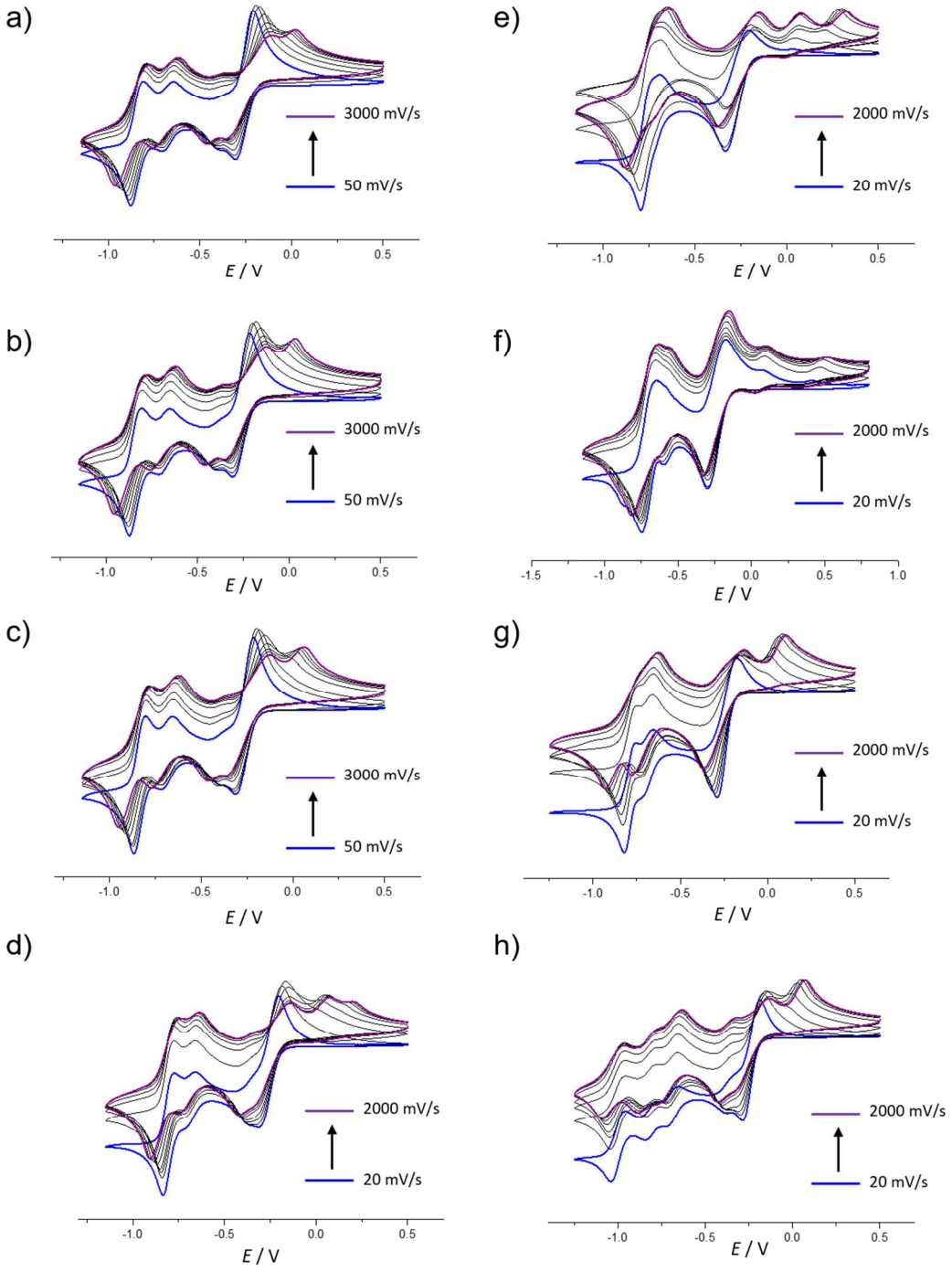


Figure S31. Normalized variable scan rate cyclic voltammograms of 1:1 mixture of CBPQT•4PF_6 and a) DB2•4PF_6, b) DB3•4PF_6, c) DB4•4PF_6, d) DB6•4PF_6, e) DB7•4PF_6, f) DB8•4PF_6, g) DB11•3PF_6, h) DB14•2PF_6 (0.5 mM in MeCN, 0.1 M TBAPF_6, 298 K), respectively.

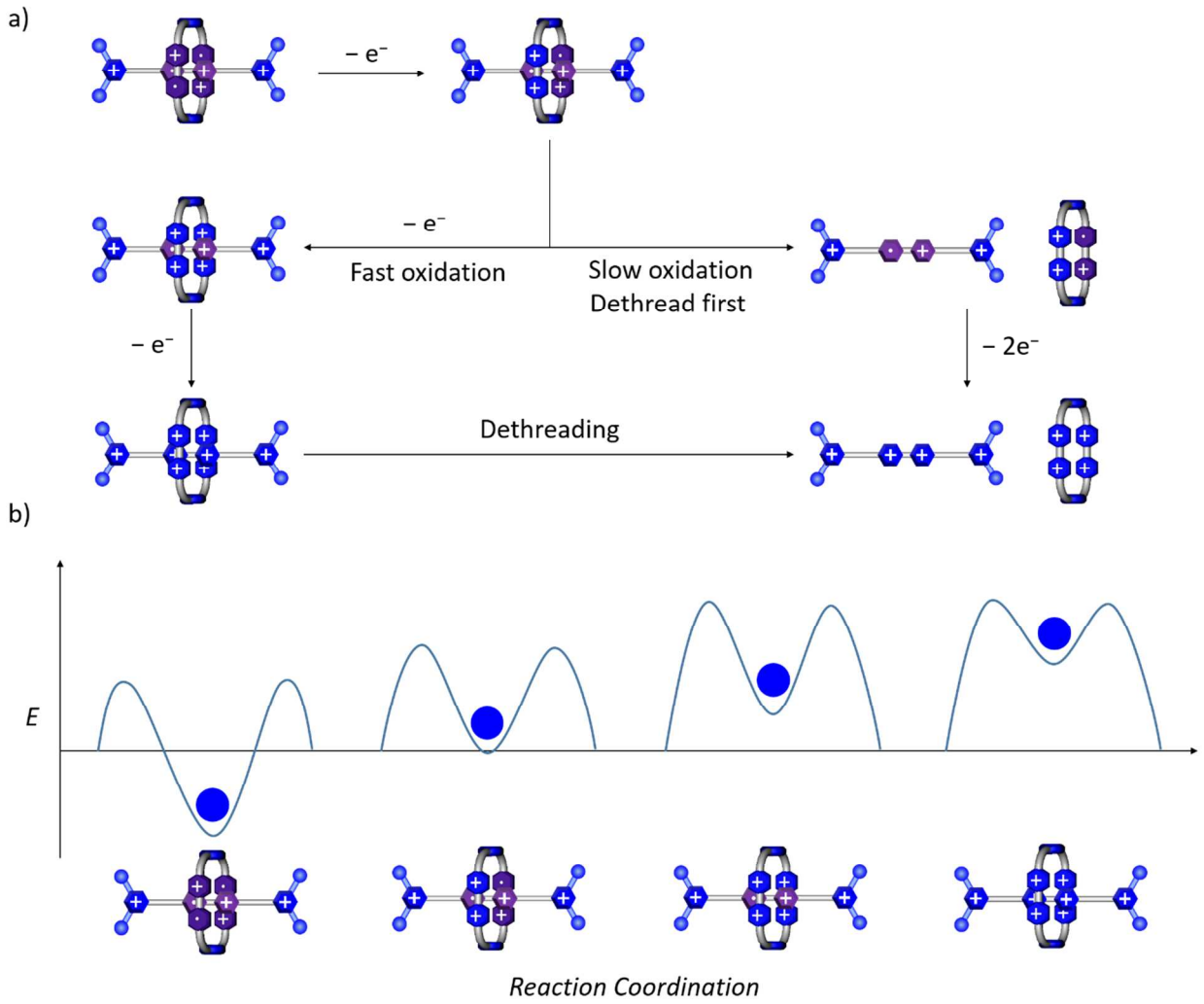


Figure S32. a) Graphical illustrations showing the different oxidation pathways under slow and fast cyclic voltammetry (CV) scan rate, respectively. b) Simplified energy surface curve of the complexes at different oxidation states.

When the dumbbell is mixed in a 1:1 molar ratio with CBPQT•4PF_6, the peak corresponding to the oxidation of the trisradical state to the fully oxidized state is split into two or three. Variable scan rate CV experiments (Figure S31) were performed and we observed the separated peak merge into one peak at low scan rates (20 mV/s). A mechanism is proposed in Figure S32 to explain the CV spectra. The trisradical complex first of all loses one electron and becomes oxidized to bisradical complex, resulting in a much weaker binding interaction. Under slow scan rate conditions, the bisradical complex disassembles in solution, followed by both $CBPQT^{+(\bullet+)}$ and $BIPY^{\bullet+}$ being oxidized separately and reveal the same oxidization peak. Under fast scan rate

conditions, however, losing another electron is faster than the bisradical complex disassembly process; on the other hand, the bisradical complex has less of a tendency to lose another electron compared with the trisradical complex on account of the increased positive charge, which makes the second oxidation peak more positive than the first one. After the complex has been oxidized to the monoradical state, the kinetic barrier for the $CBPQT^{4+}$ ring to dethread increases significantly on account of Coulombic repulsions between PY^{+} and the (increased) positive charges on $CBPQT^{4+}$ ring. As a result, losing the last electron can still be faster than the dethreading process. The cumulated positive charges make the oxidation process happened at even more positive potentials, resulting in the third oxidation peak.

6. Electron Paramagnetic Resonance (EPR) Experiments

General Procedures for EPR Experiments: In a glovebox in an atmosphere of argon, each dumbbell compound (1 mmol) was dissolved in 1 mL of MeCN and mixed with a 1 mL MeCN solution ($CBPQT{\bullet}4PF_6$ 1 mM) to afford a 1:1 dumbbell/$CBPQT^{4+}$ solution (0.5 mM). Excess of activated Zn dust was added to the mixture and it was stirred for 5 min. After filtration, the mixture was transferred to an EPR tube and sealed. Continuous wave EPR spectra were collected at X-Band (9.8 GHz) on a Bruker E580 using an ER4122SHQE resonator using non-saturating microwave power. Low temperature spectra were acquired using a liquid nitrogen finger dewar insert.

Figure S33 shows a 1:1 mixture of each dumbbell and $CBPQT{\bullet}4PF_6$ under reducing conditions. Based on the EPR spectra of $CBPQT{\bullet}4PF_6$ and a select number of the dumbbells, figure S34, the EPR spectra recorded for the mixtures don't represent a simple linear combinations of the component spectra. These results suggest that the observed EPR spectra for the mixtures of dumbbell and CBPQT•4PF6 are a result spin-spin interactions in the dumbbell/$CBPQT^{2(\bullet+)}$ complex. Low temperature EPR spectroscopy was performed on several of the complexes to gauge whether the spin-spin interaction was ferrro or anti-ferro magnetic. The absence of broad, quartet-like features in the spectrum (Figure S35) suggests that the electrons in the complex are coupled anti-ferro magnetically.

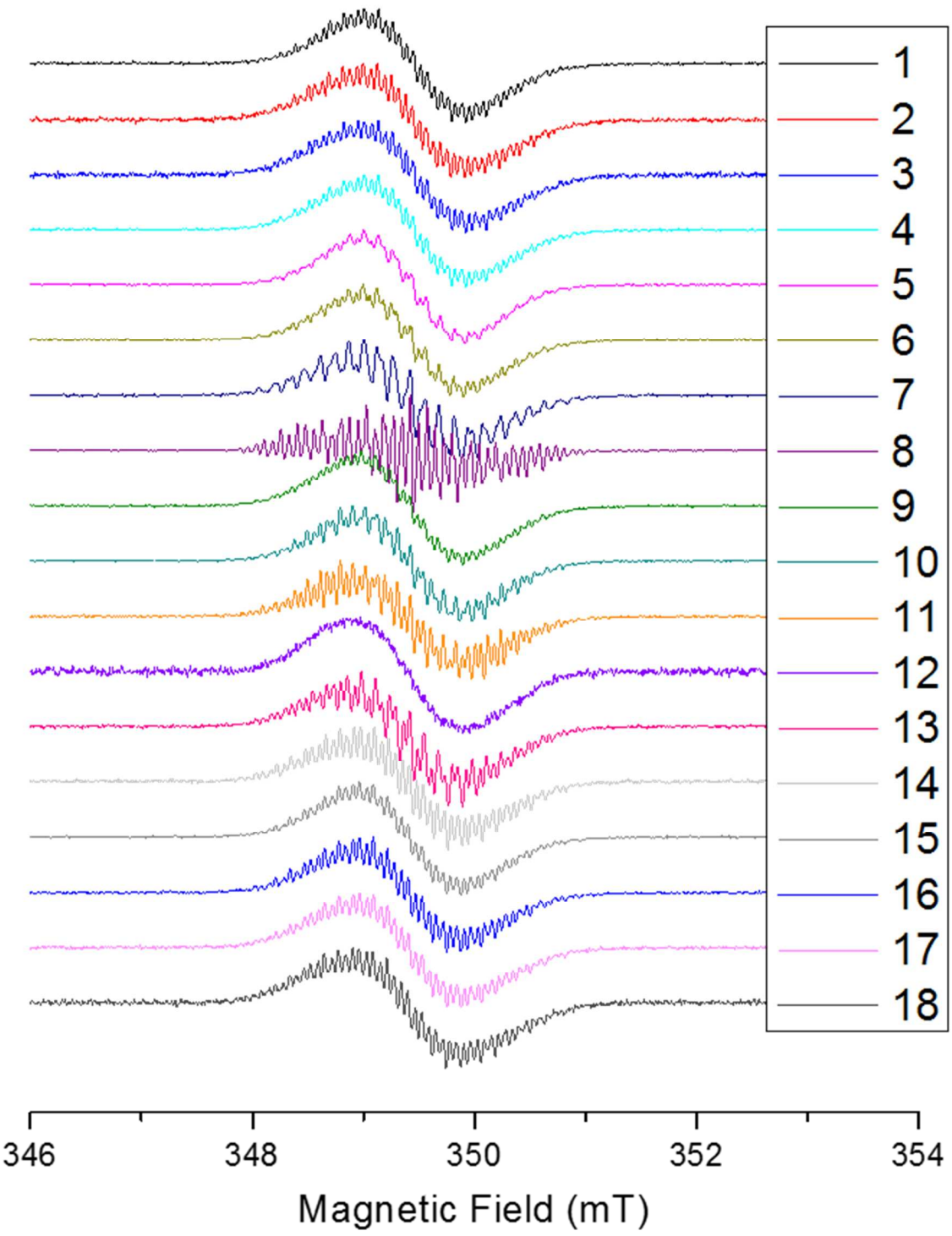


Figure S33. EPR Spectra of 1:1 mixture of each dumbbell and $CBPQT^{2(\bullet+)}$ under reducing condition.

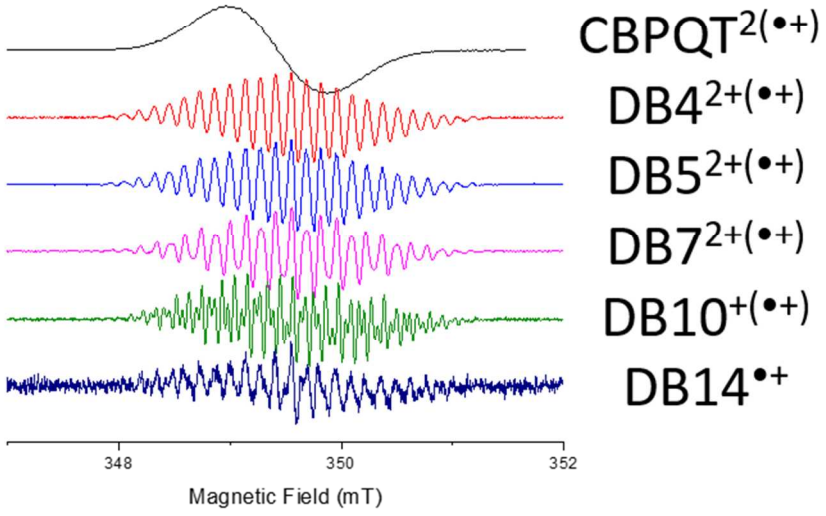


Figure S34. CW-EPR spectra of $CBPQT^{2(\bullet+)}$ and selected dumbbells.

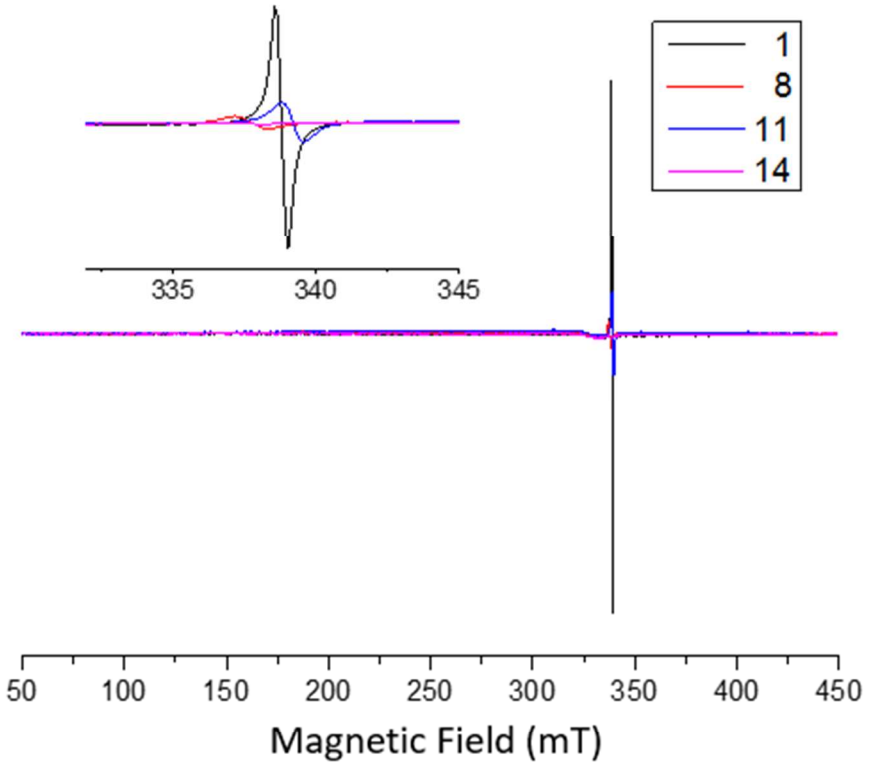
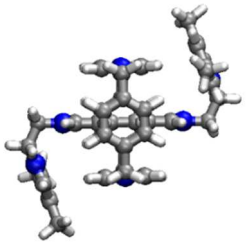
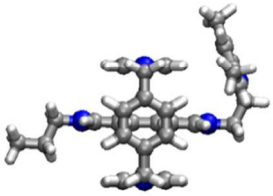
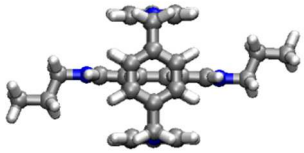
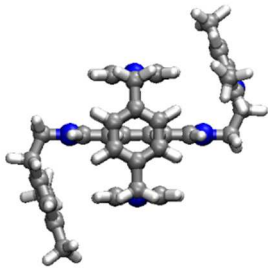
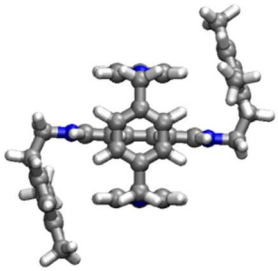


Figure S35. Low temperature EPR spectra of 1:1 mixture of $CBPQT^{2(\bullet+)}$ and selected dumbbells.

7. Density Functional Theory (DFT) Calculations

QM calculations were carried out for these systems using the Poisson-Boltzmann solvation model with the M06 density functional and the 6-311G(d,p) basis while including the D3 van der Waals corrections, which we expect to provide an accurate descriptions of the noncovalent interactions important for these systems as indicated in Table 3.

Table S3. The Structures, Charges, and Multiplicities of Complexes.

Name	Structure	Charge	Multiplicity
$DB8^{2+(\bullet+)} \subset CBPQT^{2(\bullet+)}$		5+	2
$DB9^{+(\bullet+)} \subset CBPQT^{2(\bullet+)}$		4+	2
$DB0^{\bullet+} \subset CBPQT^{2(\bullet+)}$ [a]		3+	2
$DB11^{+(\bullet+)} \subset CBPQT^{2(\bullet+)}$		4+	2
$DB14^{\bullet+} \subset CBPQT^{2(\bullet+)}$		3+	2

[a] Dumbbell structure without PY^+ or Ph.

Table S4. Comparison of the binding energies of $DB9^{+(\bullet+)}\subset CBPQT^{2(\bullet+)}$ calculated using the M06 function at a 6-311G(d,p) level with the combination of VdW corrections (D3), solvation model (Poisson-Boltzmann solvation model for MeCN), and the Wertz's approximation for the entropy fit to the experimental solvation of small molecules and explicit counterions (PF_6^-).

	VdW correction	Solvation	Liquid Correction	Counterions	Δ*G*(kcal/mol)
No VdW	N	Y	Y	N	1.10
No Solv	Y	N	Y	N	149.66
No Scale	Y	Y	N	N	1.62
With Ions	Y	Y	Y	Y	317.49
This Method[a]	Y	Y	Y	N	− 6.38
Exp					− 4.5

[a] The method we used with VdW corrections, solvation, liquid corrections and no explicit counterions gives results that best compare with the experimental data.

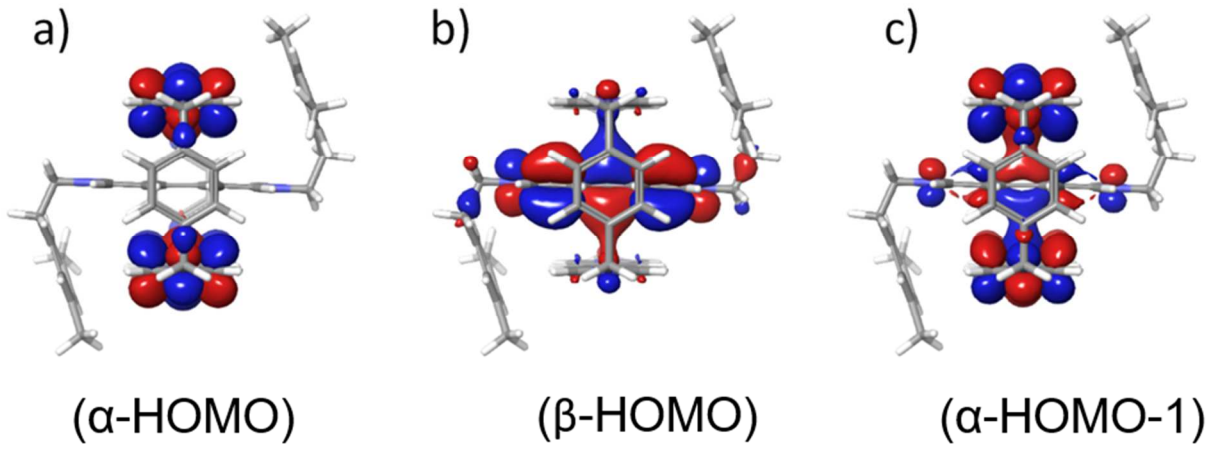


Figure S36. Frontier molecular orbitals for the HOMO levels for the 1:1 inclusion trisradical complexes between $DB14^{\bullet+}\subset CBPQT^{2(\bullet+)}$ with *S*=1/2. The doublet state has two unpaired α orbitals and one unpaired β orbital. The doublet (*S*=1/2) state is 9.0 kcal/mol more stable than the quartet (*S*=3/2) state.

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CBPQT$^{2(\bullet+)}$ E = -1609.520570 hartree

N	2.9222898798	3.5981835590	1.3382113275
N	-2.9222898798	-3.5981835590	-1.3382113275
N	-3.7081371702	2.9369606793	-1.0410134179
N	3.7081371702	-2.9369606793	1.0410134179
C	4.3055169928	3.3606445192	1.8028360732
C	-4.3055169928	-3.3606445192	-1.8028360732
C	1.8779997630	3.5166650475	2.2171430540
C	-1.8779997630	-3.5166650475	-2.2171430540
C	0.5819272623	3.5009565217	1.7921981176
C	-0.5819272623	-3.5009565217	-1.7921981176
C	0.2514728314	3.5439665345	0.3988186868
C	-0.2514728314	-3.5439665345	-0.3988186868
C	1.3756637774	3.6950565070	-0.4765123817
C	-1.3756637774	-3.6950565070	0.4765123817
C	2.6532980781	3.7060431491	0.0018363495
C	-2.6532980781	-3.7060431491	-0.0018363495
C	-1.0867416993	3.4109860909	-0.0807905767
C	1.0867416993	-3.4109860909	0.0807905767
C	-2.2071230292	3.2220997169	0.7921326838
C	2.2071230292	-3.2220997169	-0.7921326838
C	-3.4578905315	2.9831175306	0.3025516766
C	3.4578905315	-2.9831175306	-0.3025516766
C	-2.6818117145	3.1765967932	-1.9120039703
C	2.6818117145	-3.1765967932	1.9120039703
C	-1.4125955004	3.4198689138	-1.4758415476
C	1.4125955004	-3.4198689138	1.4758415476
C	-5.0013975817	2.4237040937	-1.5402671372
C	5.0013975817	-2.4237040937	1.5402671372
C	-4.9475665775	0.9125951173	-1.6548016310
C	4.9475665775	-0.9125951173	1.6548016310
C	-5.2843065264	0.1078649262	-0.5622827519
C	5.2843065264	-0.1078649262	0.5622827519
C	-5.1171054803	-1.2740745779	-0.6247571563

C	5.1171054803	1.2740745779	0.6247571563
C	-4.6103924559	-1.8753981658	-1.7807850488
C	4.6103924559	1.8753981658	1.7807850488
C	-4.3179851940	-1.0751864434	-2.8895766151
C	4.3179851940	1.0751864434	2.8895766151
C	-4.4850163671	0.3068008561	-2.8270772841
C	4.4850163671	-0.3068008561	2.8270772841
H	4.3914771382	3.7741571801	2.8122055263
H	-4.3914771382	-3.7741571801	-2.8122055263
H	4.9769462952	3.9184794640	1.1431198059
H	-4.9769462952	-3.9184794640	-1.1431198059
H	2.1400526151	3.4691842911	3.2701542333
H	-2.1400526151	-3.4691842911	-3.2701542333
H	-0.1827544055	3.4413503584	2.5578556892
H	0.1827544055	-3.4413503584	-2.5578556892
H	1.2536785985	3.7922155882	-1.5494084875
H	-1.2536785985	-3.7922155882	1.5494084875
H	3.5136554722	3.8040143395	-0.6538725210
H	-3.5136554722	-3.8040143395	0.6538725210
H	-2.1002289204	3.2483900330	1.8706828689
H	2.1002289204	-3.2483900330	-1.8706828689
H	-4.3113085207	2.8222596743	0.9548591275
H	4.3113085207	-2.8222596743	-0.9548591275
H	-2.9362098781	3.1652364205	-2.9678864199
H	2.9362098781	-3.1652364205	2.9678864199
H	-0.6622229922	3.6063988106	-2.2352089904
H	0.6622229922	-3.6063988106	2.2352089904
H	-5.1922768411	2.8941582438	-2.5094252979
H	5.1922768411	-2.8941582438	2.5094252979
H	-5.7781722614	2.7464263782	-0.8406350263
H	5.7781722614	-2.7464263782	0.8406350263
H	-5.6774671969	0.5607555870	0.3466327322
H	5.6774671969	-0.5607555870	-0.3466327322
H	-5.3818525210	-1.8861819643	0.2360796532
H	5.3818525210	1.8861819643	-0.2360796532

H	-3.9543303464	-1.5308466736	-3.8093915608
H	3.9543303464	1.5308466736	3.8093915608
H	-4.2496484428	0.9160480454	-3.6984956755
H	4.2496484428	-0.9160480454	3.6984956755

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$DB8^{2+(\bullet+)} \subset CBPQT^{2(\bullet+)}$ E = -2915.312340 hartree

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N	2.5715405470	1.9864513759	-3.5163936922
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H	2.7629335219	-5.7055192231	1.1774411764
H	1.5538711735	-6.2453555435	-0.0039554756
C	1.4375058939	-4.0206255125	-1.3299879122
H	0.8062597256	-4.8369402539	-1.6663363114
C	1.5175238806	-2.8317727809	-1.9948346735
H	0.9182532638	-2.7286543648	-2.8887112921
C	2.3586302344	-1.7730276358	-1.5350419890
C	3.1349941071	-2.0844112206	-0.3785151730
H	3.8520116737	-1.3863227079	0.0326114964
C	3.0165726996	-3.2895164949	0.2509000474
H	3.6004178206	-3.5388827943	1.1306188119
C	2.4358602362	-0.5089059496	-2.1971914196
C	1.6781271310	-0.2154633694	-3.3714075076
H	1.0177262126	-0.9456126798	-3.8176061090
C	1.7645386498	0.9965933591	-3.9873815428
H	1.2053245321	1.2287574818	-4.8851542038
C	3.3292315380	1.7481872011	-2.4069884268
H	3.9681499360	2.5622344230	-2.0799266457
C	3.2916421161	0.5481491653	-1.7583216915
H	3.9473298763	0.4346341965	-0.9053141904
C	2.4170264368	3.3669288889	-4.0271080796
H	3.3755192075	3.8772231160	-3.9141692259
H	2.1833966099	3.3100272311	-5.0932471648
C	1.3168630413	4.0410871190	-3.2351232438
C	-0.0224343050	3.8354923424	-3.5785125701
H	-0.2714671637	3.3016762966	-4.4908715291
C	-1.0442827894	4.3245074900	-2.7721531517
H	-2.0808633843	4.1675411395	-3.0617767944
C	-0.7415244331	5.0274959968	-1.6019617002
C	0.5942523869	5.2789088669	-1.2848929967
H	0.8433902535	5.8663848581	-0.4049099380
C	1.6173310665	4.7897269742	-2.0968065933
H	2.6534868919	4.9995019332	-1.8432476839
N	-2.1659735103	4.2510885478	0.2028378016
N	-2.5722173982	-1.9871454810	3.5181483190
C	-1.8512522900	5.4205460086	-0.6489931201
H	-2.7636180505	5.7041258153	-1.1776008034
H	-1.5550107946	6.2436959527	0.0045108310
C	-1.4378391082	4.0188906740	1.3292777774
H	-0.8060181605	4.8350131210	1.6650614000
C	-1.5176656056	2.8300985000	1.9942349778

H	-0.9176583997	2.7272611540	2.8877024749
C	-2.3592707804	1.7712606085	1.5349201576
C	-3.1357841865	2.0824623392	0.3783230217
H	-3.8529424962	1.3842652537	-0.0329021417
C	-3.0173111848	3.2874947330	-0.2512805991
H	-3.6011185515	3.5363991284	-1.1313285320
C	-2.4367915726	0.5070992277	2.1973476008
C	-1.6780591216	0.2136069290	3.3703944708
H	-1.0156851343	0.9428411895	3.8134301624
C	-1.7643672237	-0.9978021104	3.9874754774
H	-1.2042905103	-1.2296320715	4.8845358186
C	-3.3308196324	-1.7495085549	2.4094033308
H	-3.9703833799	-2.5634500957	2.0835920541
C	-3.2932805113	-0.5496473065	1.7597043108
H	-3.9495003629	-0.4362232979	0.9069976141
C	-2.4171907033	-3.3677829391	4.0293524096
H	-3.3757962033	-3.8781650956	3.9184643112
H	-2.1813968946	-3.3106644519	5.0946900903
C	-1.3170954438	-4.0410099256	3.2359755870
C	0.0225017352	-3.8357841718	3.5785587439
H	0.2718203756	-3.3018351113	4.4904941426
C	1.0441312681	-4.3251140218	2.7722613755
H	2.0808246844	-4.1687889482	3.0614405664
C	0.7411476578	-5.0280131581	1.6021313113
C	-0.5950628265	-5.2782524420	1.2852901269
H	-0.8444397458	-5.8651680579	0.4049806233
C	-1.6179323927	-4.7889521878	2.0975177915
H	-2.6543115758	-4.9978125118	1.8444431485
N	2.4445151943	1.1033437027	2.3318338177
C	2.0074046566	1.9346310916	1.3346813778
H	2.4750437593	2.9144224403	1.2965183507
C	1.0656988324	1.5378325623	0.4302226631
H	0.7918291525	2.2569831998	-0.3326554972
C	0.4828190777	0.2272048030	0.4731525881
C	0.9661441963	-0.5984459580	1.5393166509
H	0.6115935051	-1.6115312914	1.6794138570
C	1.9165843426	-0.1570927932	2.4118204799
H	2.3244404646	-0.7937417278	3.1896584873
C	3.4733566577	1.5519898815	3.2867976953
H	4.2517669145	2.0938516666	2.7416137432
H	3.9449806675	0.6656958088	3.7147713376
C	2.9386534369	2.4989154812	4.3640396280
H	2.5807681718	3.4301758688	3.9217738428
H	3.7414387699	2.7402529776	5.0654979703
C	1.9194406873	0.7068598498	5.7051875323
H	2.8646564068	0.1877995242	5.5677709278
C	0.8803185558	0.1560128166	6.4457617898
C	-0.2688451608	0.9280104190	6.6268491758
H	-1.0951431231	0.5293648158	7.2154513844
C	-0.3805198956	2.2047462039	6.0710322711
C	0.6925794528	2.6774939727	5.3262896323
H	0.6981604253	3.6693780876	4.8820004322
C	1.0111094216	-1.2163705841	7.0470076485

H	1.5182272814	-1.1544402451	8.0139818085
H	1.5992206500	-1.8797976758	6.4094413231
H	0.0260369942	-1.6564383238	7.2208712027
C	-1.6117049184	3.0429327953	6.2755119907
H	-2.4829729295	2.4054925809	6.4376328574
H	-1.4841569583	3.6728813783	7.1606563834
H	-1.8052962109	3.6961657392	5.4226942858
N	-2.4440904099	-1.1026151003	-2.3316366189
C	-2.0068234930	-1.9338194641	-1.3347891243
H	-2.4747270514	-2.9134158868	-1.2963879955
C	-1.0646379194	-1.5371384482	-0.4306156249
H	-0.7906312367	-2.2562042819	0.3321058624
C	-0.4816636262	-0.2266112687	-0.4738773983
C	-0.9651256261	0.5990259623	-1.5398589511
H	-0.6105670810	1.6122372597	-1.6800629996
C	-1.9161907082	0.1576227826	-2.4120452046
H	-2.3247463922	0.7942972912	-3.1897847686
C	-3.4732284819	-1.5514354929	-3.2864498390
H	-4.2502710955	-2.0947256635	-2.7408642472
H	-3.9461646869	-0.6653154635	-3.7137131537
C	-2.9376440928	-2.4971810890	-4.3641339651
H	-2.5792584405	-3.4280940378	-3.9219177843
H	-3.7397680497	-2.7385112276	-5.0662696787
C	-1.9194150945	-0.7052650348	-5.7060379127
H	-2.8653996141	-0.1868314785	-5.5694499266
C	-0.8802874032	-0.1547475818	-6.4473534536
C	0.2693412483	-0.9262754590	-6.6277659770
H	1.0949647936	-0.5289422315	-7.2182934514
C	0.3818813587	-2.2020819604	-6.0701855126
C	-0.6907027008	-2.6741031540	-5.3243388201
H	-0.6958422953	-3.6650985621	-4.8785421736
C	-1.0121675241	1.2166255850	-7.0504959117
H	-1.5185451859	1.1529689828	-8.0181038827
H	-1.6015226093	1.8801087979	-6.4137426245
H	-0.0270620709	1.6570625101	-7.2242166531
C	1.6125174529	-3.0406105853	-6.2755754651
H	2.4835706268	-2.4031588169	-6.4383568330
H	1.4839190493	-3.6696274999	-7.1612059747
H	1.8065473719	-3.6944877177	-5.4234415664
N	1.8032589923	1.9294532871	5.1495018612
N	-1.8023049267	-1.9269694951	-5.1489534558

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DB82+(•+) E=-1305.764580 hartree

N	0.1379898858	1.9784900659	2.9412853179
C	-0.9499309942	2.0405327597	2.1121289559
H	-1.7360561985	2.7310563413	2.4023073421
C	-1.0271572348	1.2897622892	0.9781377528
H	-1.9192005422	1.4091720797	0.3766752031
C	0.0247729312	0.3951553044	0.5957936121
C	1.1378436969	0.3646662766	1.4944767718
H	1.9984208484	-0.2677610179	1.3167433943
C	1.1706186242	1.1442427236	2.6103318722

H	2.0280250269	1.1576272201	3.2740652604
C	0.1991809444	2.8053695250	4.1558630603
H	-0.1570108371	3.8107053888	3.9149132330
H	1.2465366449	2.8988460681	4.4481784574
C	-0.6740426626	2.2782231849	5.2976480390
H	-1.7286922500	2.2986848721	5.0202362768
H	-0.5371694002	2.9075664244	6.1807741217
C	0.9105130908	0.5253541127	5.9717887509
H	1.6598195822	1.3104330757	5.9188724479
C	1.2304961351	-0.7730567815	6.3326421328
C	0.1857355050	-1.6916371171	6.4406863522
H	0.4052437533	-2.7167436088	6.7349321050
C	-1.1326877138	-1.3221718223	6.1852836807
C	-1.3684874731	-0.0150350726	5.7849225096
H	-2.3637308466	0.3499627672	5.5480883293
C	2.6547132764	-1.1653267706	6.6133889474
H	2.9161608648	-0.9326824373	7.6499547726
H	3.3498406077	-0.6328485768	5.9611633587
H	2.7860923914	-2.2383951677	6.4633804157
C	-2.2682681197	-2.2920018770	6.3574194469
H	-1.9221758906	-3.3150508114	6.2007570987
H	-2.6618805977	-2.2225750631	7.3764418781
H	-3.0842995514	-2.0829244740	5.6634465418
N	-0.1376066361	-1.9776694307	-2.9407231800
C	0.9503371092	-2.0399344023	-2.1113329287
H	1.7359039631	-2.7312263193	-2.4013661121
C	1.0277934423	-1.2891902114	-0.9773778775
H	1.9196766784	-1.4091960050	-0.3756619077
C	-0.0240939585	-0.3944020736	-0.5950394733
C	-1.1369787244	-0.3635315636	-1.4941411673
H	-1.9974663304	0.2690158773	-1.3164368515
C	-1.1698993931	-1.1428370017	-2.6101168367
H	-2.0270268164	-1.1554901890	-3.2743115465
C	-0.1987183846	-2.8045932687	-4.1548927683
H	0.1580571624	-3.8095321226	-3.9136043147
H	-1.2461693588	-2.8986309707	-4.4467181451
C	0.6742906948	-2.2781389738	-5.2972107109
H	1.7290704038	-2.2979712289	-5.0200949035
H	0.5382107300	-2.9081184991	-6.1799877325
C	-0.9110714314	-0.5253326070	-5.9711201757
H	-1.6607507604	-1.3099319095	-5.9168844054
C	-1.2311700815	0.7728040544	-6.3327706584
C	-0.1863638936	1.6912303206	-6.4412656748
H	-0.4058410240	2.7164984492	-6.7350747730
C	1.1319605969	1.3211953185	-6.1865382129
C	1.3682830337	0.0142116956	-5.7862751512
H	2.3638942541	-0.3509854706	-5.5506627006
C	-2.6553705584	1.1649844887	-6.6137580011
H	-2.9168491599	0.9315661195	-7.6501525954
H	-3.3507883096	0.6334684702	-5.9611158176
H	-2.7859031376	2.2382755280	-6.4649448193
C	2.2679420114	2.2901848266	-6.3592102973
H	1.9221617051	3.3132906198	-6.2029005672

H	2.6623047891	2.2201894126	-7.3778651527
H	3.0834054865	2.0801028695	-5.6650053162
N	-0.3606928591	0.8736756289	5.6882546606
N	0.3603374983	-0.8739711188	-5.6884416605

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$DB9^{+(\bullet+)} \subset CBPQT^{2(\bullet+)}$ E= -2628.518317 hartree

N	2.4532506204	-4.2270151168	0.8183389553
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H	3.1128370746	-5.0030790787	2.6444182823
H	1.9663497382	-6.0296998047	1.7603186463
C	1.7333254759	-4.4866737596	-0.3103494668
H	1.1594901401	-5.4075877639	-0.3098799691
C	1.7548836432	-3.6416176051	-1.3805190122
H	1.1758347976	-3.9347524380	-2.2455083449
C	2.5222176242	-2.4357351257	-1.3615794806
C	3.2916452798	-2.2313159371	-0.1747818564
H	3.9553336076	-1.3842528883	-0.0616345194
C	3.2347973663	-3.1099627821	0.8670208842
H	3.8162338779	-2.9693057997	1.7722510155
C	2.5374030828	-1.5182576045	-2.4575733094
C	1.8014696640	-1.7483412449	-3.6606743895
H	1.2269918070	-2.6515352319	-3.8160282708
C	1.8124375581	-0.8449111823	-4.6827931000
H	1.2644323754	-1.0085993403	-5.6047702031
C	3.2791526152	0.5566568976	-3.4922829934
H	3.8541528251	1.4766374876	-3.4951014143
C	3.3084677746	-0.3153486071	-2.4438834025
H	3.9484358380	-0.0553489756	-1.6112173500
C	2.3076239240	1.3883926504	-5.5930882614
H	3.2329183016	1.9612242695	-5.6825150425
H	2.0911125999	0.9205554239	-6.5558826159
C	1.1562919944	2.2432907611	-5.1070373091
C	-0.1610007662	1.8411817273	-5.3483407002
H	-0.3615882066	0.9853267471	-5.9887039031
C	-1.2234871455	2.5350242440	-4.7789904730
H	-2.2424840660	2.2151539878	-4.9833155255
C	-0.9868673825	3.6410774245	-3.9570067558
C	0.3252509345	4.0735107171	-3.7584791227
H	0.5211349863	4.9600854920	-3.1606873461
C	1.3906661667	3.3792965244	-4.3310720928
H	2.4077101985	3.7299504767	-4.1744865133
N	-2.3984832219	3.5130586470	-1.9849327745
N	-2.4923036169	-1.0360170044	3.4340743626
C	-2.1366279361	4.2913054663	-3.2161707087
H	-3.0540163108	4.2968921053	-3.8082753801
H	-1.9038750283	5.3166440390	-2.9217667221
C	-1.6760566692	3.7645612574	-0.8585534322
H	-1.0950321402	4.6809420438	-0.8604601187
C	-1.6995770176	2.9129698848	0.2060740128
H	-1.1069767716	3.1886170417	1.0669815270
C	-2.4722249207	1.7110581271	0.1864916403

C	-3.2454121516	1.5169973163	-0.9987105504
H	-3.9128282833	0.6731759980	-1.1131583828
C	-3.1853810513	2.4002266802	-2.0363671216
H	-3.7660187898	2.2633997686	-2.9425368251
C	-2.4860227590	0.7881267664	1.2738887631
C	-1.7254450264	0.9997343979	2.4651558952
H	-1.1077324349	1.8778705676	2.5925944909
C	-1.7474606180	0.1034664581	3.4894958885
H	-1.1825152159	0.2545600713	4.4006251433
C	-3.2475863186	-1.2758094933	2.3221386371
H	-3.8314881919	-2.1903813216	2.3297824960
C	-3.2724787460	-0.4066574746	1.2717220395
H	-3.9208637507	-0.6618996940	0.4438950335
C	-2.2627591794	-2.1141176619	4.4202627745
H	-3.1850428500	-2.6910160685	4.5101109745
H	-2.0547573313	-1.6493291501	5.3868767025
C	-1.1070812282	-2.9640025380	3.9368582173
C	0.2093537839	-2.5622184323	4.1806180017
H	0.4044419294	-1.7122578265	4.8278886830
C	1.2770173544	-3.2504337379	3.6151672186
H	2.2957401470	-2.9318054517	3.8249314491
C	1.0439390921	-4.3552285922	2.7901982273
C	-0.2672214035	-4.7898290169	2.5889144232
H	-0.4602915378	-5.6755534111	1.9891346306
C	-1.3360856436	-4.0993378116	3.1592095233
H	-2.3517291095	-4.4521944203	2.9997252778
N	2.3600284845	1.7019523753	1.1667750689
C	1.8926729036	2.0702517818	-0.0694614524
H	2.3024149135	2.9904115899	-0.4746877238
C	0.9959178025	1.3048065878	-0.7541822849
H	0.6936438183	1.6655256557	-1.7300950392
C	0.4909367594	0.0733699043	-0.2193146075
C	1.0014083970	-0.2618080725	1.0762601738
H	0.7068477385	-1.1699231261	1.5866633012
C	1.9055940480	0.5313364911	1.7165864429
H	2.3355102475	0.2580080949	2.6743525527
C	3.3408516452	2.5381471557	1.8752265751
H	4.0948595556	2.8839473499	1.1623167978
H	3.8571047077	1.9095787681	2.6031661333
C	2.7328725022	3.7860177110	2.5205117909
H	2.3308262867	4.4599131482	1.7626951234
H	3.5050072686	4.3203652314	3.0799397037
C	1.7934202683	2.5707171194	4.4386729677
H	2.7715965473	2.1009393230	4.5050201731
C	0.7730972015	2.2723081716	5.3334557029
C	-0.4266243311	2.9756702169	5.2095086175
H	-1.2415253579	2.7735388745	5.9040896451
C	-0.6032448532	3.9384024396	4.2131990484
C	0.4573743772	4.1667789554	3.3456292502
H	0.4137691814	4.9174869419	2.5612692391
C	0.9810784310	1.2414512223	6.4088570062
H	1.4612635268	1.6992601561	7.2786388967
H	1.6273093522	0.4307225203	6.0652300779

H	0.0244790849	0.8296548544	6.7392902432
C	-1.8851376718	4.7128878574	4.0846755096
H	-2.7227219599	4.1297243830	4.4715383414
H	-1.8169782293	5.6361942800	4.6672867060
H	-2.0916398102	4.9846256025	3.0480382137
N	-2.3145815811	-2.3734993153	-2.2778557960
C	-1.8491696586	-2.7394259416	-1.0512658817
H	-2.2601897081	-3.6588477802	-0.6457184241
C	-0.9346927971	-1.9833046645	-0.3754550637
H	-0.6230575323	-2.3468269064	0.5961047120
C	-0.4282015874	-0.7620136570	-0.9229938549
C	-0.9214720010	-0.4427983203	-2.2260089581
H	-0.6011533420	0.4451380963	-2.7557674643
C	-1.8333023371	-1.2406747942	-2.8581030386
H	-2.2267014214	-1.0105759987	-3.8431796565
C	-3.2983656570	-3.2250912270	-2.9770887308
H	-4.0669573735	-3.5077238710	-2.2522750951
H	-3.7701308406	-2.6080795980	-3.7449285154
C	-2.6534179443	-4.4625126348	-3.5957582501
H	-2.2081047218	-5.0755548800	-2.8060761346
H	-1.8449977829	-4.1527489029	-4.2650511643
C	-3.6913207579	-5.2767742057	-4.3655553279
H	-3.2425127251	-6.1784208636	-4.7851321883
H	-4.1106393511	-4.6935454429	-5.1894793210
H	-4.5139080829	-5.5816756361	-3.7132069616
N	1.6158124076	3.4834801229	3.4637588782

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DB9+(•+) E=-1018.961728 hartree

N	0.3870537389	-2.0138060613	1.7242782744
C	-0.6863765401	-2.3686197714	0.9451604413
H	-1.3905611551	-3.0669075596	1.3867751978
C	-0.8420055007	-1.8872621140	-0.3186200057
H	-1.7115516626	-2.2308689077	-0.8644037271
C	0.1041062506	-0.9795257905	-0.9006356107
C	1.2061159719	-0.6388720611	-0.0499523345
H	1.9950802987	0.0280401804	-0.3745382038
C	1.3227472058	-1.1566339753	1.2031408965
H	2.1767069002	-0.9379673576	1.8348111432
C	0.5390090230	-2.5578450629	3.0781566248
H	0.3032944817	-3.6257440903	3.0591050495
H	1.5891435190	-2.4653686210	3.3612238373
C	-0.3928973992	-1.9104891355	4.1058432113
H	-1.4369577090	-2.1201282127	3.8692686579
H	-0.1748377243	-2.3118048293	5.0991397620
C	0.9570236757	0.1235808817	4.3713726399
H	1.7929768451	-0.5601435129	4.4933238812
C	1.1153671301	1.4998570271	4.4292167486
C	-0.0333638557	2.2883002016	4.3289695725
H	0.0584391154	3.3721347486	4.3797181354
C	-1.2954038866	1.7169129306	4.1707682799
C	-1.3671573466	0.3335119307	4.0742106353
H	-2.3066203487	-0.1913535624	3.9275915674

C	2.4789500444	2.1080876400	4.6125312205
H	2.7337986541	2.1529654356	5.6757507556
H	3.2458187573	1.5198793904	4.1041646245
H	2.4948371456	3.1243463058	4.2147626780
C	-2.5438086672	2.5541949557	4.1306278576
H	-2.3241402227	3.5485771236	3.7388300673
H	-2.9405309976	2.6704569433	5.1441351289
H	-3.3163108484	2.0909818454	3.5144037723
N	-0.3178915209	0.5836224892	-4.8329551173
C	0.7338629551	0.9580446197	-4.0508146897
H	1.4236619163	1.6753792776	-4.4855021957
C	0.9001448031	0.4636980237	-2.7903547692
H	1.7612853538	0.8178742964	-2.2390955458
C	-0.0295693320	-0.4670717764	-2.2271425443
C	-1.1028522537	-0.8414385417	-3.0941436769
H	-1.8655913718	-1.5466194714	-2.7904818645
C	-1.2155548352	-0.3188098264	-4.3502223183
H	-2.0257312734	-0.5918782294	-5.0179731059
C	-0.4549358611	1.1323411620	-6.1946937860
H	-0.2611952266	2.2071381592	-6.1390840210
H	-1.4947415085	0.9900445315	-6.4969306809
C	0.4934539356	0.4576256070	-7.1824763701
H	1.5266454483	0.6222994049	-6.8632105113
H	0.3189305031	-0.6217893644	-7.1652042343
C	0.2857005227	1.0055317974	-8.5924976558
H	0.9844171063	0.5435994205	-9.2918961984
H	-0.7287046838	0.8017128928	-8.9449782870
H	0.4449220664	2.0868402102	-8.6222821123
N	-0.2587503003	-0.4272168938	4.1747918908

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$DB0^{(\bullet+)} \subset CBPQT^{2(\bullet+)}$ E= -2341.722172 hartree

N	2.9462467511	-1.2319164209	3.5670140518
N	2.8251911791	-1.6619056140	-3.4896412989
C	2.6836383892	-1.0009340805	5.0025750927
H	3.4985896232	-0.3905915304	5.3976234282
H	2.6970639489	-1.9702601784	5.5054729805
C	2.4332972349	-2.3357528136	2.9517946470
H	2.0391521875	-3.1065044765	3.6057952826
C	2.4332031946	-2.4613942189	1.5946357342
H	2.0256892123	-3.3771101662	1.1889039234
C	2.9585643666	-1.4327341369	0.7513414360
C	3.5237590909	-0.3175178044	1.4457143392
H	4.0018276291	0.5001285323	0.9228561254
C	3.4982664596	-0.2428364634	2.8064653496
H	3.9236719979	0.5969729643	3.3458016158
C	2.9346097238	-1.5199337635	-0.6722737803
C	2.4059311381	-2.6535083041	-1.3665376308
H	2.0415790754	-3.5254635412	-0.8407488342
C	2.3598808583	-2.6939121840	-2.7280998771
H	1.9659377405	-3.5480948048	-3.2683429595
C	3.3764630737	-0.5764818898	-2.8729825348
H	3.7566372443	0.2024275158	-3.5256297675

C	3.4524827298	-0.4872518642	-1.5154220325
H	3.9272214185	0.3967291097	-1.1108769851
C	2.5139724149	-1.6072978580	-4.9324659166
H	3.3101220858	-1.0468695511	-5.4267401811
H	2.5171107766	-2.6304417758	-5.3142165538
C	1.1647114266	-0.9441718716	-5.1099952748
C	-0.0052471319	-1.6960710869	-4.9700619866
H	0.0513375692	-2.7757433555	-4.8536713551
C	-1.2478198432	-1.0717792800	-4.9823967951
H	-2.1484129797	-1.6707411965	-4.8715835880
C	-1.3425005781	0.3140715626	-5.1387138879
C	-0.1772517478	1.0585384336	-5.3284858140
H	-0.2386705426	2.1313714987	-5.4935346117
C	1.0690412405	0.4333061284	-5.3135960984
H	1.9688820399	1.0241937444	-5.4657531160
N	-2.9445947426	1.2323194167	-3.5594572140
N	-2.8238490026	1.6680731812	3.4966442298
C	-2.6837902242	1.0016880036	-4.9947175440
H	-3.4984422596	0.3904044249	-5.3890689548
H	-2.6981819246	1.9706547695	-5.4980380779
C	-2.4321472062	2.3371983524	-2.9441297953
H	-2.0384912601	3.1080034331	-3.5983051406
C	-2.4329084496	2.4637205545	-1.5873884125
H	-2.0280276659	3.3808838141	-1.1822894076
C	-2.9574997579	1.4349048612	-0.7433656663
C	-3.5219678373	0.3188186173	-1.4373852094
H	-4.0003785529	-0.4983236632	-0.9139797167
C	-3.4962842409	0.2431096907	-2.7978449007
H	-3.9214652025	-0.5971173974	-3.3367207866
C	-2.9340349104	1.5234714453	0.6804782044
C	-2.4047696744	2.6571227157	1.3728749654
H	-2.0394528076	3.5280665472	0.8462121544
C	-2.3585010107	2.6990048363	2.7347501913
H	-1.9640722072	3.5536786285	3.2739827768
C	-3.3766298884	0.5831186497	2.8820707670
H	-3.7579763650	-0.1945250282	3.5357088053
C	-3.4527166667	0.4923182148	1.5241858583
H	-3.9281311239	-0.3918065315	1.1207497721
C	-2.5118419881	1.6142523693	4.9401897534
H	-3.3085018828	1.0551993216	5.4353645747
H	-2.5135410845	2.6375887351	5.3213031101
C	-1.1629426235	0.9489784405	5.1153839686
C	0.0087233838	1.7014284138	4.9885979843
H	-0.0463566024	2.7826962409	4.8843590722
C	1.2511914464	1.0760956874	5.0033210839
H	2.1539769579	1.6757659639	4.9122947092
C	1.3426264285	-0.3121173815	5.1437439953
C	0.1757052571	-1.0570907151	5.3218221645
H	0.2349016760	-2.1313839811	5.4785489630
C	-1.0697369090	-0.4302700530	5.3082046083
H	-1.9706829739	-1.0212031264	5.4539709671
N	1.6976533368	3.0888506413	-0.2429990960
C	1.3312596215	2.4095662871	-1.3674300930

H	1.6139646014	2.8700020779	-2.3091221792
C	0.6647461957	1.2217834841	-1.3023876326
H	0.4142253306	0.7485945322	-2.2439652536
C	0.3245654202	0.6296654049	-0.0453659173
C	0.6970079977	1.3985722758	1.1010537905
H	0.4732530296	1.0677027184	2.1070907548
C	1.3599431636	2.5853367077	0.9768942871
H	1.6572485801	3.1820599707	1.8331409675
C	2.3958969274	4.3810490848	-0.3663457231
H	3.1631961411	4.2703077463	-1.1379750800
H	2.8992783053	4.5733299210	0.5837552423
C	1.4341733616	5.5141275447	-0.7134101572
N	-1.7068975189	-3.0919560105	0.2486522737
C	-1.3399384670	-2.4155829628	1.3748421043
H	-1.6228992272	-2.8775437247	2.3157540105
C	-0.6720461621	-1.2278838574	1.3115006034
H	-0.4204182938	-0.7562667278	2.2536540690
C	-0.3324422404	-0.6330717222	0.0554438188
C	-0.7071732433	-1.3990010350	-1.0922948444
H	-0.4884836000	-1.0643657639	-2.0977650245
C	-1.3696354771	-2.5852253030	-0.9700632924
H	-1.6681511057	-3.1789622758	-1.8277271424
C	-2.3984518958	-4.3883187662	0.3607051795
H	-3.1694369672	-4.2909190046	1.1302475891
H	-2.8967225667	-4.5738109989	-0.5934860931
C	-1.4307204768	-5.5194912032	0.6966782863
H	-0.9519445202	-5.3128074345	1.6590924946
H	-0.6410533608	-5.5525317101	-0.0607377575
C	-2.1627209328	-6.8578195412	0.7535769897
H	-1.4775327250	-7.6619377217	1.0263857211
H	-2.6026995335	-7.1027923104	-0.2166698393
H	-2.9664391907	-6.8330181863	1.4945779334
H	0.6918679558	5.6123027120	0.0844220124
H	0.8945768543	5.2617050904	-1.6318091563
C	2.1891194959	6.8277503414	-0.8996278309
H	2.7210524957	7.1075240655	0.0131863275
H	1.5009044890	7.6362546646	-1.1503002964
H	2.9212384537	6.7451869228	-1.7074231459

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DB0(•+) E=-732.158379 hartree

N	0.4497690390	0.1701831324	3.5063595880
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H	0.6246612502	-1.9056407546	3.4786035051
C	0.2824407640	-1.1206088386	1.5104225767
H	0.3069746503	-2.1133200213	1.0805772393
C	0.0786441595	0.0460427396	0.7065097238
C	0.0576415204	1.2777571827	1.4341323843
H	-0.0982287623	2.2291610713	0.9424962088
C	0.2385628775	1.3075624159	2.7852767090
H	0.2270382042	2.2328830658	3.3504761155
C	0.6304069213	0.2129622119	4.9668556757
H	1.4588232109	-0.4547466492	5.2167104511

H	0.9259260842	1.2304290519	5.2291180957
C	-0.6367492779	-0.1931155186	5.7150297123
N	-0.4584687060	-0.1499445991	-3.5064423745
C	-0.4709615166	1.0533935080	-2.8616507747
H	-0.6349331256	1.9260413816	-3.4854888297
C	-0.2922767912	1.1468905138	-1.5143047422
H	-0.3169270267	2.1406468908	-1.0867125542
C	-0.0879037368	-0.0174382473	-0.7070456085
C	-0.0655000609	-1.2509514985	-1.4311383871
H	0.0911552013	-2.2011125674	-0.9375541949
C	-0.2459956890	-1.2847245643	-2.7818054790
H	-0.2325952574	-2.2117646691	-3.3440487812
C	-0.6326347037	-0.2051292448	-4.9673950832
H	-1.4621160807	0.4567511642	-5.2288530261
H	-0.9224879162	-1.2266343380	-5.2202341336
C	0.6378033096	0.1949422240	-5.7132225483
H	0.9022216228	1.2223154474	-5.4479428057
H	1.4600407884	-0.4444177137	-5.3807695011
C	0.4477591330	0.0738602574	-7.2221352816
H	1.3483967260	0.3888877781	-7.7513573977
H	0.2328803571	-0.9596013613	-7.5060284217
H	-0.3808740367	0.6993675928	-7.5650525179
H	-1.4396918516	0.5028982330	5.4582514142
H	-0.9511103678	-1.1843687669	5.3765771181
C	-0.4023513697	-0.2061800433	7.2225440403
H	-0.0985132033	0.7805237221	7.5815752290
H	-1.3122354142	-0.4919705834	7.7525627420
H	0.3817265639	-0.9201429056	7.4884898303

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$DB11^{+(\bullet+)} \subset CBPQT^{2(\bullet+)}$ E=-2898.849113 hartree

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H	2.7486381702	-5.7105899141	1.1752349497
H	1.5401284563	-6.2558282292	-0.0027834665
C	1.4162127172	-4.0304838437	-1.3364145181
H	0.7783991126	-4.8440355554	-1.6656082066
C	1.4954713007	-2.8446300538	-2.0057095375
H	0.8852787924	-2.7370106061	-2.8925851962
C	2.3484213822	-1.7902975545	-1.5543040807
C	3.1334438910	-2.1031510563	-0.4027448357
H	3.8560917489	-1.4070657505	0.0021993302
C	3.0129473900	-3.3047263091	0.2316603567
H	3.6019943852	-3.5551920112	1.1075584871
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H	0.8408455948	5.8574415370	-0.4457258961
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C	-1.7710782158	-0.9908138038	3.9647110168
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H	-3.9772848768	-0.4208765380	0.9014568837
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H	2.3330607702	-0.7896858596	3.1792770837
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C	-0.9728770292	0.5779369013	-1.5422046465
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C	0.2810025279	-0.9429314931	-6.6237453151
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DB11+(•+) E=-1289.286234 hartree

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H	-1.7249233786	2.3191361410	5.0003373793
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$DB14^{\bullet+} \subset CBPQT^{2(\bullet+)}$ E=-2882.385686 hartree

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C	-3.0114372013	3.2971287806	-0.2552176887
H	-3.6001210031	3.5410266778	-1.1336660044
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C	-0.3848072319	2.2347816434	6.0313044508
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H	1.5120420611	-1.1068974177	8.0125977041
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